



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 01:03 AM JST

PDB ID : 9WQ8 / pdb_00009wq8
EMDB ID : EMD-66162
Title : Structure of yeast Pol II in complex with a longer scaffold containing a cisplatin-ICL lesion at +7 position.
Authors : Xu, J.; Zhu, L.
Deposited on : 2025-09-10
Resolution : 2.98 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

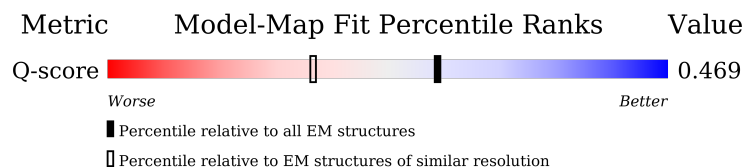
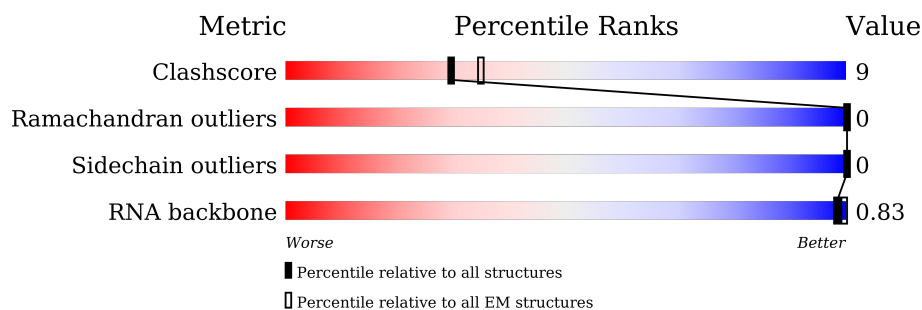
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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 $\leq 5\%$. 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	A	1733	
2	B	1224	
3	C	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	18	
14	P	6	
15	T	25	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1423	Total	C	N	O	S	0	0
			11197	7055	1957	2124	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1183	Total	C	N	O	S	0	0
			9421	5955	1648	1762	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	165	Total	C	N	O	S	0	0
			1326	820	237	267	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	139	Total	C	N	O	S	0	0
			1113	699	187	223	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a DNA chain called DNA (NTS, non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	15	Total	C	N	O	P	0	0
			321	149	73	84	15		

- Molecule 14 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	6	Total	C	N	O	P	0	0
			135	60	30	39	6		

- Molecule 15 is a DNA chain called DNA (TS, template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	22	Total	C	N	O	P	0	0
			430	208	59	141	22		

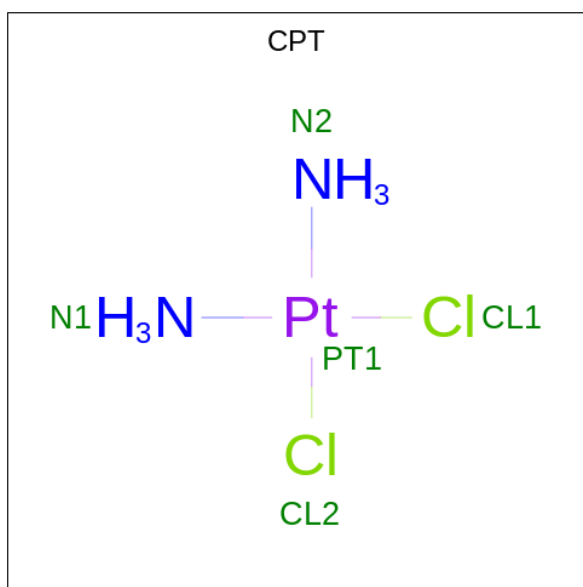
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is Cisplatin (CCD ID: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$) (labeled as "Ligand of Interest" by depositor).

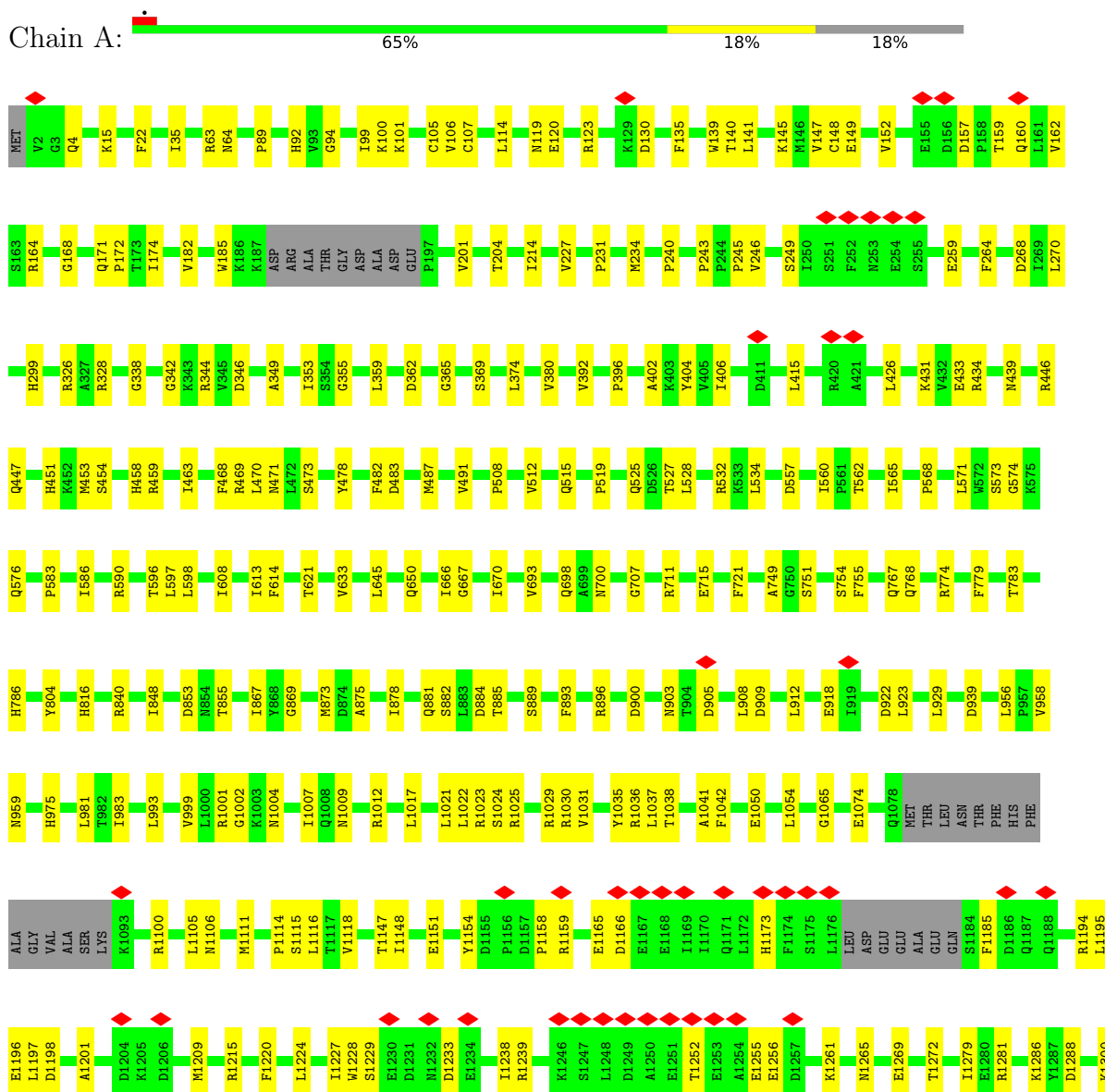


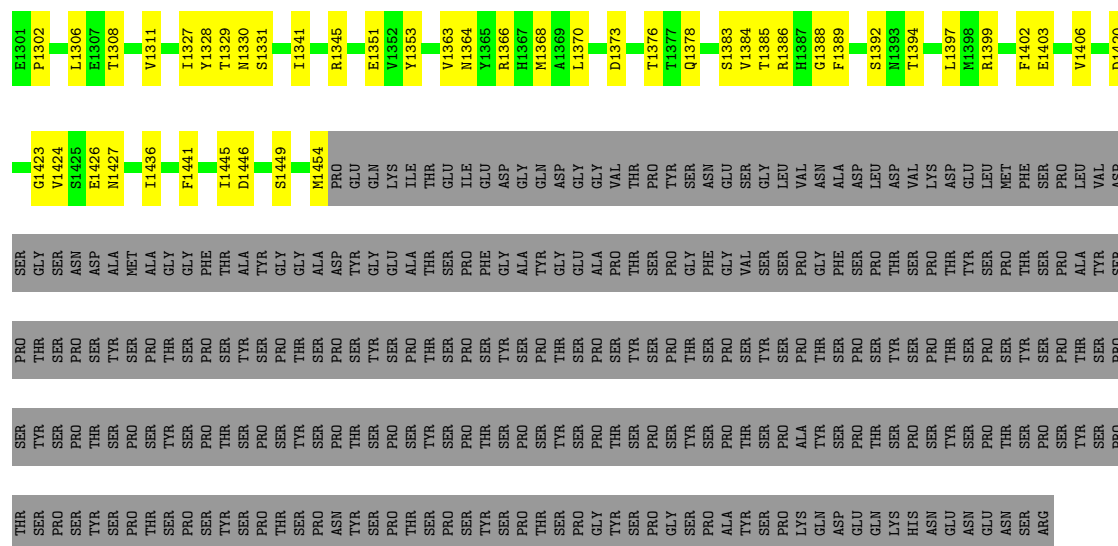
Mol	Chain	Residues	Atoms			AltConf
18	T	1	Total	N	Pt	0
			3	2	1	

3 Residue-property plots

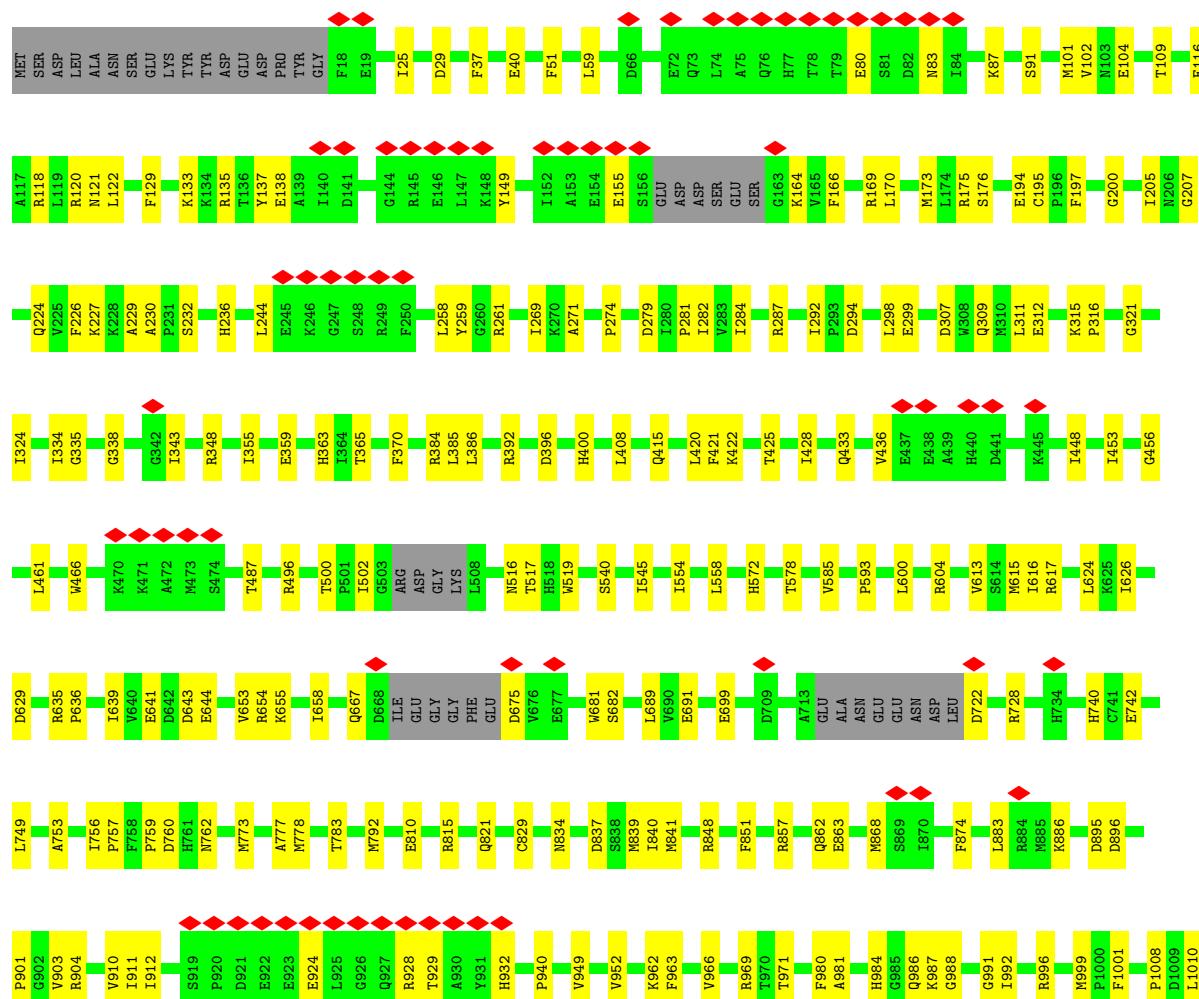
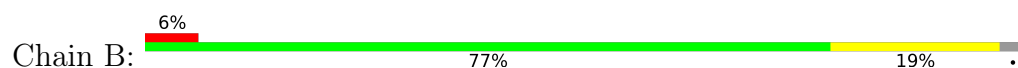
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 II subunit RPB1

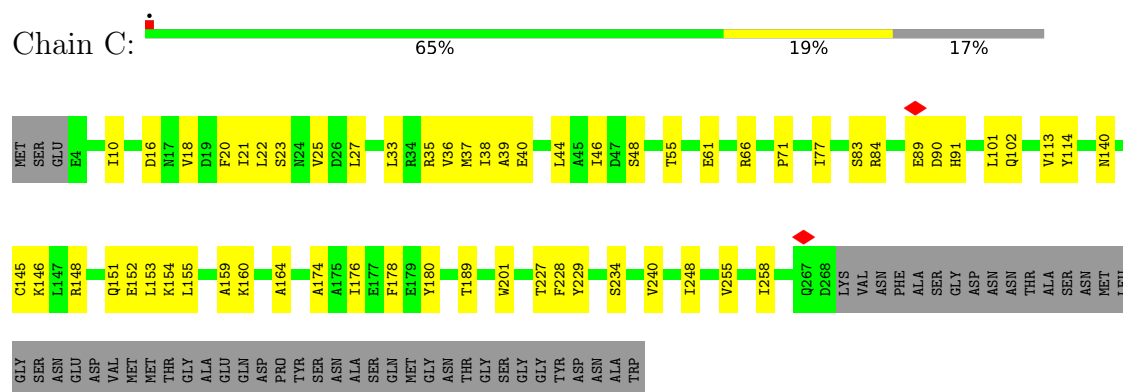




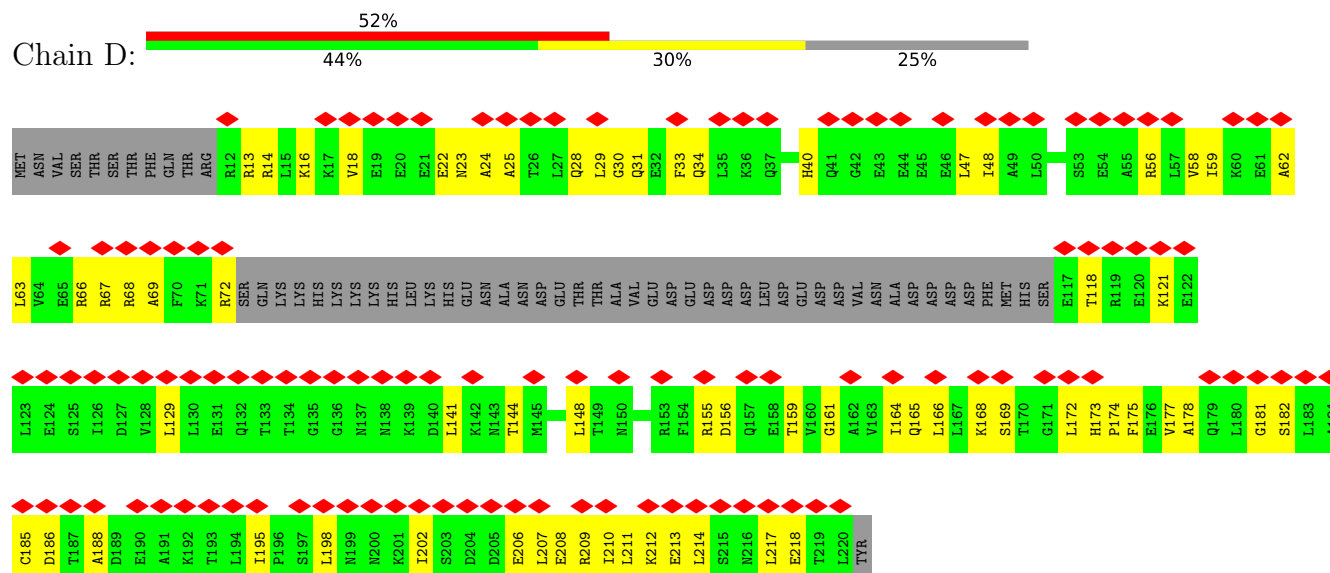
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



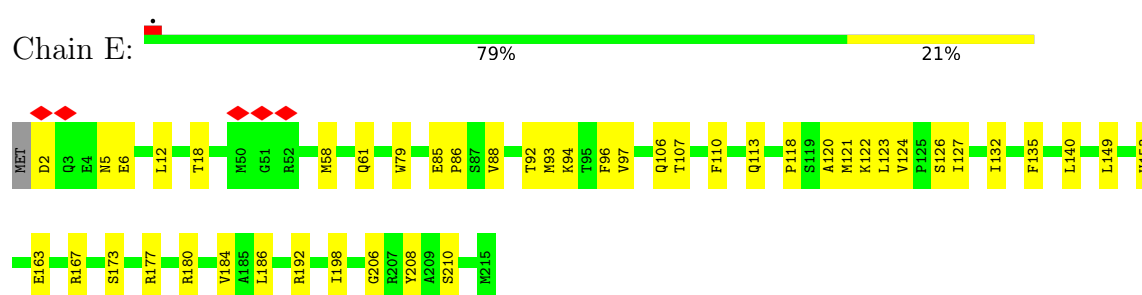
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



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



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



MET SER ASP TYR GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU ASP PHE ASP VAL HIS PHE SER ASP GLU THR GLU LYS PRO GLN PHE LYS ASP GLY THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR L69 T81 M85 E89 R97 Q100 D116 R119 E127 K128 K129 V133 R136 W146 S147 V148 D154 L155

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

Chain G: 53% 65% 35%

M1 I4 K5 D6 T12 L13 H14 P15 F18 L26 E35 T39 Q100 F42 G43 Y44 L45 L46 C47 Y48 L49 D50 Y51 I61 L62 P63 T64 D65 A68 K73 Y74 R75 A76 V77 V78 F79 K80 P81 F82 K83 G84 E85 V86 V87 D88 G89 V92 V93 C94 S95 Q96 H97 G98 F99 E100 V101 Q102 V103 G104 P105 M106 K107 V108 F109 V110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120 F121 M122 A123 G124 S125 M126 P127 P128 S129 Y130 Q131 S132 S133 E134 D135 V136 I137 T138 T139 K140 S141 R142 I143 V145 K146 I147 E148 G149 C150 I151 S152 Q153 V154 S155 S156 I157 H158 A159 I160 G161 S162 I163 K164 E165 D166 Y167 L168 G169 A170 I171

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

Chain H: 75% 21% 5%

MET S2 D7 F10 A28 T32 Q33 C36 L46 S61 S62 L63 D67 T68 PRO ALA ASN ASP SER A75 T76 S77 S78 P82 D86 R87 S88 L89 A101 Y102 K103 F104 S108 K109 Y116 S117 F118 G119 L122 M123 R124 L125 E126 L135 K136 Q137 L142 R146 K146

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

Chain I: 7% 66% 29% 5%

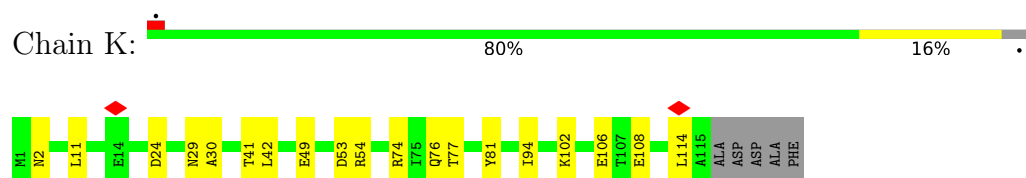
MET T2 T3 F4 R5 F6 C7 L14 R17 E18 E21 N22 N23 R24 L25 L26 C29 Y34 E37 A38 G39 L42 R45 I52 G60 D61 R73 E74 K77 C78 R81 Q87 F101 V102 C103 C106 S107 H108 T111 S112 D113 Q114 K115 N116 K117 ARG THR GLN PHE SER

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

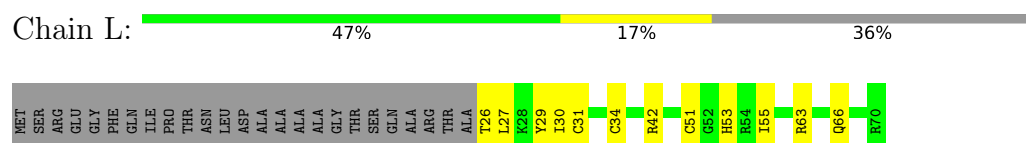
Chain J: 73% 26%

H1 I2 V3 C7 V13 Y21 L25 L41 Y44 C45 R47 R48 M49 T52 I57 E58 R62 L66 E67 R68 R69 ASP

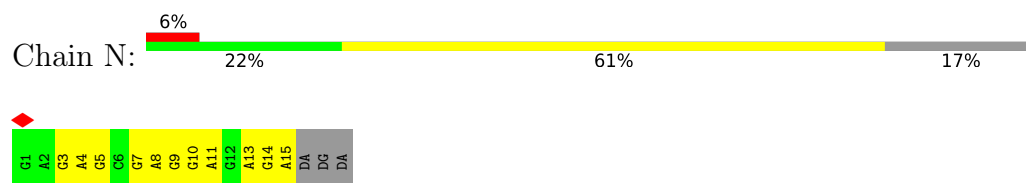
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



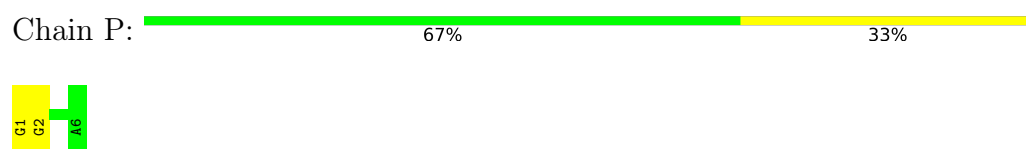
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



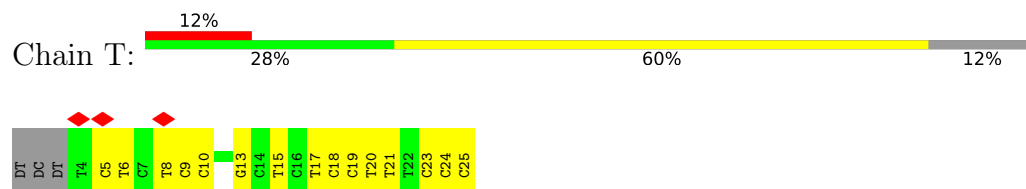
- Molecule 13: DNA (NTS, non-template strand)



- Molecule 14: RNA (5'-R(P*GP*GP*GP*AP*AP*A)-3')



- Molecule 15: DNA (TS, template strand)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63622	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)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.683	Depositor
Minimum map value	-0.404	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	3/11398 (0.0%)	0.31	1/15413 (0.0%)
2	B	0.17	0/9607	0.30	0/12958
3	C	0.18	0/2124	0.30	0/2879
4	D	0.13	0/1334	0.32	0/1789
5	E	0.16	0/1788	0.32	0/2406
6	F	0.17	0/717	0.30	0/967
7	G	0.16	0/1367	0.36	0/1844
8	H	0.17	0/1131	0.26	0/1532
9	I	0.13	0/962	0.30	0/1295
10	J	0.18	0/578	0.28	0/775
11	K	0.17	0/942	0.26	0/1272
12	L	0.14	0/361	0.30	0/478
13	N	0.61	0/364	0.93	0/562
14	P	0.70	0/152	0.83	0/236
15	T	0.65	0/474	0.99	0/725
All	All	0.22	3/33299 (0.0%)	0.35	1/45131 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	PRO	N-CD	-8.56	1.35	1.47
1	A	240	PRO	N-CD	-7.63	1.37	1.47
1	A	249	SER	C-N	-7.08	1.25	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLN	CB-CA-C	-5.53	110.22	116.63

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	11197	0	11268	207	0
2	B	9421	0	9421	170	0
3	C	2086	0	2045	44	0
4	D	1326	0	1348	50	0
5	E	1752	0	1776	32	0
6	F	705	0	731	8	0
7	G	1339	0	1357	44	0
8	H	1113	0	1079	21	0
9	I	944	0	899	29	0
10	J	569	0	585	12	0
11	K	924	0	934	17	0
12	L	359	0	381	11	0
13	N	321	0	166	10	0
14	P	135	0	66	1	0
15	T	430	0	252	20	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	T	3	0	0	0	0
All	All	32633	0	32308	584	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 9.

All (584) 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)
9:I:78:CYS:SG	9:I:106:CYS:HB3	1.95	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:8:DT:H1'	15:T:9:DC:H5'	1.44	0.99
13:N:13:DA:N1	15:T:6:DT:N3	2.17	0.93
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.19	0.81
1:A:469:ARG:NH2	2:B:991:GLY:O	2.16	0.79
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.68	0.75
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.69	0.74
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.20	0.74
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.21	0.73
15:T:5:DC:H1'	15:T:6:DT:H5''	1.72	0.72
4:D:211:LEU:HA	4:D:214:LEU:HB2	1.72	0.72
1:A:562:THR:O	1:A:576:GLN:NE2	2.21	0.71
2:B:928:ARG:NH1	2:B:929:THR:O	2.23	0.71
15:T:9:DC:H2''	15:T:10:DC:H5''	1.73	0.71
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.23	0.70
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.72	0.70
4:D:62:ALA:HB2	7:G:49:LEU:HD13	1.74	0.70
2:B:792:MET:SD	2:B:857:ARG:NH2	2.65	0.70
7:G:83:LYS:HG3	7:G:148:GLU:HA	1.74	0.70
10:J:48:ARG:NH1	10:J:49:MET:SD	2.65	0.69
1:A:700:ASN:O	9:I:115:LYS:NZ	2.25	0.69
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.65	0.69
2:B:309:GLN:HE22	9:I:52:ILE:HD11	1.57	0.69
9:I:74:GLU:OE1	9:I:81:ARG:NH2	2.26	0.69
1:A:1215:ARG:NH2	1:A:1272:THR:O	2.26	0.68
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.26	0.68
5:E:2:ASP:HB2	5:E:5:ASN:HB3	1.75	0.68
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.28	0.67
2:B:129:PHE:HB3	2:B:164:LYS:HB2	1.76	0.67
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.77	0.67
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.67
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.28	0.67
15:T:5:DC:H1'	15:T:6:DT:C5'	2.25	0.66
1:A:157:ASP:OD1	1:A:160:GLN:NE2	2.28	0.66
4:D:14:ARG:NH1	4:D:16:LYS:O	2.29	0.66
1:A:1166:ASP:OD2	1:A:1239:ARG:NH1	2.29	0.66
5:E:106:GLN:HG2	5:E:107:THR:HG23	1.77	0.66
4:D:24:ALA:N	7:G:83:LYS:O	2.22	0.65
1:A:909:ASP:HB3	1:A:912:LEU:HG	1.79	0.65
2:B:487:THR:OG1	2:B:777:ALA:O	2.14	0.65
7:G:106:MET:HE3	7:G:157:ILE:HG23	1.77	0.65
1:A:119:ASN:O	1:A:123:ARG:NH1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:ALA:O	2:B:261:ARG:NH1	2.30	0.64
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.30	0.64
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.78	0.64
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.79	0.64
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.32	0.64
15:T:17:DT:H2'	15:T:18:DC:C6	2.34	0.63
2:B:307:ASP:OD2	2:B:392:ARG:NH1	2.30	0.63
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.32	0.63
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.34	0.63
1:A:1384:VAL:HA	1:A:1389:PHE:HD1	1.64	0.63
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.30	0.63
5:E:2:ASP:O	5:E:6:GLU:N	2.28	0.63
1:A:896:ARG:HD2	1:A:1030:ARG:HH11	1.62	0.63
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.27	0.62
4:D:141:LEU:HA	7:G:46:LEU:HD12	1.81	0.62
1:A:64:ASN:HD22	2:B:924:GLU:HB2	1.62	0.62
10:J:48:ARG:O	10:J:52:THR:OG1	2.17	0.62
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.17	0.62
1:A:359:LEU:O	1:A:471:ASN:ND2	2.32	0.62
7:G:127:PRO:HG2	7:G:139:ILE:HG12	1.81	0.62
15:T:13:DG:H2''	15:T:15:DT:C4	2.34	0.62
2:B:135:ARG:HD3	2:B:155:GLU:HG3	1.80	0.61
4:D:214:LEU:O	4:D:218:GLU:N	2.33	0.61
1:A:568:PRO:HD2	8:H:46:LEU:HG	1.83	0.61
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.82	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.81	0.61
1:A:355:GLY:O	1:A:469:ARG:NH1	2.34	0.61
7:G:132:SER:OG	7:G:135:ASP:OD1	2.19	0.61
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.83	0.60
1:A:560:ILE:H	8:H:78:SER:HB2	1.66	0.60
3:C:71:PRO:HG3	10:J:13:VAL:HG21	1.82	0.60
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.83	0.60
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.65	0.60
2:B:496:ARG:NH1	2:B:540:SER:O	2.25	0.60
1:A:246:VAL:O	1:A:328:ARG:NH2	2.32	0.60
1:A:147:VAL:HG13	1:A:149:GLU:HG2	1.83	0.60
2:B:773:MET:HE1	2:B:987:LYS:HE3	1.84	0.60
7:G:79:PHE:HE2	7:G:106:MET:HG2	1.67	0.59
13:N:5:DG:N2	13:N:7:DG:C2	2.70	0.59
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.35	0.59
2:B:901:PRO:HA	2:B:949:VAL:HG13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ARG:NH1	3:C:174:ALA:O	2.32	0.59
13:N:14:DG:H2'	13:N:15:DA:C8	2.37	0.59
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.84	0.59
15:T:9:DC:H4'	15:T:10:DC:OP1	2.00	0.59
7:G:46:LEU:HD21	7:G:105:PRO:HG3	1.85	0.59
1:A:63:ARG:NE	1:A:63:ARG:O	2.36	0.59
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.32	0.59
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.85	0.59
15:T:24:DC:H2'	15:T:25:DC:C6	2.38	0.58
3:C:38:ILE:HG12	3:C:176:ILE:HD12	1.85	0.58
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.37	0.58
4:D:166:LEU:O	4:D:169:SER:OG	2.17	0.58
1:A:4:GLN:HB3	2:B:1159:ARG:NH2	2.19	0.58
12:L:26:THR:OG1	12:L:27:LEU:N	2.37	0.58
7:G:79:PHE:CD2	7:G:105:PRO:HD2	2.39	0.58
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.86	0.57
2:B:101:MET:HE2	2:B:109:THR:HG22	1.86	0.57
2:B:904:ARG:NH1	12:L:66:GLN:O	2.37	0.57
1:A:596:THR:OG1	1:A:598:LEU:O	2.18	0.57
1:A:939:ASP:OD2	1:A:1023:ARG:NE	2.33	0.57
9:I:5:ARG:HH12	9:I:39:GLY:H	1.53	0.57
7:G:144:ARG:NH1	7:G:171:ILE:HG13	2.19	0.57
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.85	0.57
3:C:89:GLU:HG2	3:C:90:ASP:H	1.70	0.57
3:C:83:SER:HB3	3:C:160:LYS:HG2	1.87	0.57
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.85	0.57
8:H:82:PRO:O	11:K:54:ARG:NH2	2.38	0.57
4:D:174:PRO:HA	4:D:177:VAL:HG22	1.86	0.57
7:G:125:SER:HB3	7:G:131:GLN:HB2	1.86	0.57
1:A:140:THR:HG23	1:A:141:LEU:HD12	1.86	0.56
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.87	0.56
4:D:29:LEU:HD11	4:D:175:PHE:CD1	2.40	0.56
3:C:36:VAL:HG13	3:C:40:GLU:HB2	1.85	0.56
4:D:22:GLU:OE1	7:G:83:LYS:N	2.38	0.56
4:D:210:ILE:O	4:D:214:LEU:N	2.24	0.56
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.39	0.56
4:D:14:ARG:HH12	4:D:18:VAL:H	1.53	0.56
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.87	0.56
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.87	0.56
7:G:47:CYS:SG	7:G:48:VAL:N	2.77	0.56
2:B:80:GLU:OE1	2:B:83:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:NH2	1:A:1351:GLU:OE1	2.26	0.55
2:B:500:THR:HG22	2:B:502:ILE:HG12	1.87	0.55
2:B:986:GLN:NE2	2:B:1022:THR:OG1	2.39	0.55
2:B:91:SER:HB3	2:B:133:LYS:HB3	1.88	0.55
2:B:312:GLU:OE1	2:B:315:LYS:NZ	2.39	0.55
3:C:89:GLU:HG2	3:C:90:ASP:N	2.21	0.55
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.88	0.55
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.87	0.55
1:A:1115:SER:OG	1:A:1330:ASN:OD1	2.20	0.55
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.89	0.55
2:B:1041:GLU:N	2:B:1041:GLU:OE1	2.40	0.55
1:A:473:SER:OG	1:A:650:GLN:NE2	2.40	0.55
4:D:14:ARG:HH22	4:D:18:VAL:H	1.55	0.55
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.89	0.54
2:B:667:GLN:HE22	2:B:675:ASP:HA	1.71	0.54
2:B:952:VAL:HG12	2:B:966:VAL:HG13	1.90	0.54
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.71	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.54
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.25	0.54
1:A:1030:ARG:HH21	1:A:1035:TYR:HH	1.53	0.54
2:B:422:LYS:HA	2:B:425:THR:HG22	1.89	0.54
5:E:120:ALA:O	5:E:124:VAL:N	2.40	0.54
1:A:439:ASN:OD1	1:A:459:ARG:NH1	2.37	0.54
1:A:1173:HIS:NE2	1:A:1228:TRP:O	2.38	0.54
1:A:1329:THR:HG22	1:A:1331:SER:H	1.72	0.54
3:C:10:ILE:HA	3:C:20:PHE:HA	1.89	0.54
10:J:7:CYS:HA	10:J:49:MET:HG3	1.90	0.54
2:B:25:ILE:HA	2:B:655:LYS:HD3	1.90	0.54
1:A:365:GLY:N	1:A:469:ARG:O	2.25	0.54
1:A:975:HIS:CD2	1:A:1036:ARG:HD2	2.43	0.54
2:B:104:GLU:OE2	2:B:120:ARG:NH2	2.27	0.54
5:E:153:HIS:CG	5:E:184:VAL:HG11	2.43	0.54
1:A:101:LYS:NZ	13:N:8:DA:OP2	2.39	0.54
1:A:528:LEU:HD23	1:A:751:SER:HA	1.90	0.54
2:B:51:PHE:HB2	2:B:173:MET:HE3	1.90	0.53
2:B:641:GLU:OE2	2:B:654:ARG:NH2	2.40	0.53
2:B:287:ARG:NH1	2:B:321:GLY:O	2.41	0.53
1:A:396:PRO:HD3	1:A:415:LEU:HB3	1.91	0.53
4:D:59:ILE:HD11	7:G:77:VAL:HG21	1.89	0.53
9:I:17:ARG:N	9:I:26:LEU:O	2.35	0.53
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.89	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.89	0.53
6:F:81:THR:OG1	6:F:146:TRP:NE1	2.42	0.53
1:A:101:LYS:HD3	1:A:135:PHE:HE2	1.73	0.53
1:A:767:GLN:NE2	1:A:768:GLN:O	2.41	0.53
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.91	0.53
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.89	0.53
4:D:155:ARG:H	4:D:159:THR:HG21	1.74	0.53
1:A:981:LEU:HD11	1:A:1042:PHE:HB2	1.91	0.52
4:D:118:THR:HG23	4:D:121:LYS:H	1.74	0.52
4:D:185:CYS:SG	4:D:186:ASP:N	2.82	0.52
1:A:227:VAL:HG11	4:D:14:ARG:HA	1.91	0.52
8:H:108:SER:OG	8:H:109:LYS:N	2.42	0.52
1:A:882:SER:O	1:A:1025:ARG:NH2	2.40	0.52
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.90	0.52
1:A:1147:THR:HG21	1:A:1195:LEU:HD23	1.92	0.52
4:D:161:GLY:HA2	4:D:164:ILE:HG22	1.92	0.52
12:L:51:CYS:SG	12:L:53:HIS:HB2	2.50	0.52
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.91	0.52
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.92	0.52
2:B:839:MET:O	2:B:991:GLY:N	2.42	0.52
2:B:1163:CYS:HB2	2:B:1187:ASN:HD21	1.73	0.52
5:E:173:SER:HB2	5:E:177:ARG:HH21	1.76	0.52
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.45	0.52
1:A:1001:ARG:HH22	1:A:1054:LEU:HD22	1.74	0.51
1:A:114:LEU:O	1:A:164:ARG:NH2	2.40	0.51
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.43	0.51
2:B:334:ILE:O	2:B:338:GLY:N	2.44	0.51
5:E:79:TRP:HD1	5:E:96:PHE:HE1	1.58	0.51
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.91	0.51
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.50	0.51
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.40	0.51
5:E:180:ARG:HH21	5:E:192:ARG:HB3	1.76	0.51
4:D:14:ARG:HH22	4:D:18:VAL:N	2.08	0.51
2:B:315:LYS:HG3	2:B:316:PRO:HD3	1.93	0.51
1:A:707:GLY:HA2	1:A:1281:ARG:HD3	1.93	0.51
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.46	0.51
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.93	0.51
15:T:23:DC:H2'	15:T:24:DC:C6	2.45	0.51
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.93	0.50
1:A:402:ALA:HA	1:A:434:ARG:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.45	0.50
1:A:451:HIS:O	1:A:454:SER:OG	2.23	0.50
2:B:116:GLU:HG3	12:L:55:ILE:HD11	1.93	0.50
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.26	0.50
2:B:722:ASP:OD1	2:B:722:ASP:N	2.43	0.50
2:B:778:MET:HE1	2:B:1098:MET:HE2	1.93	0.50
1:A:881:GLN:NE2	1:A:958:VAL:O	2.43	0.50
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.93	0.50
3:C:16:ASP:O	3:C:234:SER:N	2.43	0.50
5:E:18:THR:OG1	5:E:140:LEU:O	2.19	0.50
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.50
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.94	0.50
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.93	0.50
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.45	0.50
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.92	0.50
5:E:198:ILE:HB	5:E:210:SER:HB3	1.94	0.49
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.49
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.95	0.49
1:A:1151:GLU:OE2	9:I:45:ARG:NH1	2.45	0.49
1:A:1328:TYR:HD1	5:E:149:LEU:HD11	1.77	0.49
2:B:173:MET:O	2:B:176:SER:OG	2.21	0.49
2:B:298:LEU:HD12	9:I:6:PHE:CZ	2.47	0.49
3:C:35:ARG:NE	11:K:41:THR:OG1	2.29	0.49
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.94	0.49
5:E:120:ALA:HA	5:E:123:LEU:HG	1.92	0.49
9:I:24:ARG:NH2	9:I:37:GLU:OE2	2.44	0.49
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.94	0.49
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.94	0.49
4:D:30:GLY:O	4:D:34:GLN:NE2	2.42	0.49
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.78	0.49
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.93	0.49
2:B:636:PRO:HA	2:B:691:GLU:O	2.11	0.49
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.95	0.49
7:G:116:PRO:HD2	7:G:119:LEU:HB3	1.95	0.49
1:A:1384:VAL:HA	1:A:1389:PHE:CD1	2.44	0.49
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.44	0.49
9:I:2:THR:HG22	9:I:42:LEU:HG	1.93	0.49
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.78	0.49
1:A:900:ASP:OD2	1:A:903:ASN:ND2	2.46	0.49
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.46	0.49
1:A:106:VAL:HG11	1:A:214:ILE:HG12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HB2	1:A:433:GLU:HB3	1.94	0.49
1:A:1159:ARG:HE	1:A:1185:PHE:HB2	1.78	0.49
1:A:1165:GLU:OE1	1:A:1194:ARG:NH2	2.45	0.49
2:B:895:ASP:HB2	12:L:27:LEU:HD11	1.95	0.49
1:A:869:GLY:HA3	1:A:1366:ARG:NH1	2.28	0.48
2:B:87:LYS:HE2	2:B:137:TYR:HB2	1.95	0.48
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.48	0.48
5:E:93:MET:HG2	5:E:120:ALA:HB1	1.95	0.48
1:A:470:LEU:HD21	1:A:482:PHE:HE1	1.78	0.48
1:A:565:ILE:HG21	8:H:46:LEU:HD23	1.94	0.48
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.93	0.48
2:B:903:VAL:HG22	12:L:63:ARG:HD3	1.95	0.48
8:H:86:ASP:O	8:H:87:ARG:NH1	2.46	0.48
2:B:138:GLU:N	2:B:138:GLU:OE1	2.46	0.48
4:D:188:ALA:HA	4:D:207:LEU:CD2	2.43	0.48
7:G:143:ILE:HD11	7:G:163:ILE:HG21	1.94	0.48
13:N:5:DG:C2	13:N:7:DG:C2	3.01	0.48
1:A:380:VAL:HG21	1:A:426:LEU:HD12	1.95	0.48
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.96	0.48
2:B:311:LEU:HB3	9:I:4:PHE:CE2	2.48	0.48
2:B:1122:ARG:N	15:T:23:DC:OP1	2.45	0.48
2:B:1129:ARG:HG2	15:T:21:DT:H5''	1.94	0.48
3:C:23:SER:HA	3:C:227:THR:HA	1.96	0.48
4:D:144:THR:HA	7:G:104:GLY:HA2	1.96	0.48
3:C:48:SER:OG	12:L:66:GLN:OE1	2.31	0.48
5:E:88:VAL:HG21	5:E:110:PHE:HE2	1.78	0.48
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.48
5:E:120:ALA:O	5:E:124:VAL:HG23	2.14	0.48
9:I:77:LYS:HD3	9:I:108:HIS:CG	2.49	0.48
11:K:24:ASP:OD2	11:K:74:ARG:NE	2.36	0.48
9:I:5:ARG:HH12	9:I:38:ALA:HA	1.79	0.48
1:A:908:LEU:HA	1:A:1029:ARG:HH12	1.77	0.48
3:C:66:ARG:NH1	10:J:3:VAL:O	2.42	0.48
3:C:180:TYR:HB3	3:C:228:PHE:CD2	2.49	0.48
13:N:10:DG:H2''	13:N:11:DA:H5'	1.95	0.48
5:E:12:LEU:HG	5:E:58:MET:HE1	1.94	0.48
13:N:5:DG:C2	13:N:7:DG:N1	2.82	0.48
1:A:1154:TYR:OH	9:I:18:GLU:OE2	2.23	0.47
1:A:1454:MET:SD	1:A:1454:MET:N	2.87	0.47
7:G:110:VAL:HG13	7:G:161:GLY:O	2.13	0.47
1:A:532:ARG:HD3	1:A:749:ALA:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:SER:OG	8:H:119:GLY:O	2.27	0.47
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.95	0.47
5:E:126:SER:OG	5:E:127:ILE:N	2.46	0.47
11:K:77:THR:OG1	11:K:81:TYR:O	2.27	0.47
4:D:213:GLU:O	4:D:217:LEU:N	2.35	0.47
7:G:74:TYR:CE2	7:G:76:ALA:HB2	2.49	0.47
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.96	0.47
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.49	0.47
7:G:144:ARG:HH21	7:G:167:TYR:C	2.22	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.47
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.96	0.47
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.95	0.47
2:B:653:VAL:HA	2:B:689:LEU:HD12	1.96	0.47
5:E:121:MET:HE2	5:E:124:VAL:HG21	1.96	0.47
10:J:67:GLU:HG2	12:L:30:ILE:HG12	1.95	0.47
1:A:130:ASP:OD1	1:A:130:ASP:N	2.48	0.47
1:A:369:SER:N	11:K:2:ASN:OD1	2.41	0.47
2:B:384:ARG:NH2	2:B:396:ASP:OD2	2.48	0.47
7:G:12:THR:HA	7:G:68:ALA:O	2.15	0.47
7:G:39:THR:HG23	7:G:42:PHE:H	1.80	0.47
12:L:31:CYS:SG	12:L:34:CYS:N	2.77	0.47
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.49	0.47
3:C:152:GLU:OE1	10:J:69:ARG:NH1	2.48	0.47
11:K:114:LEU:H	11:K:114:LEU:HD23	1.79	0.47
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.29	0.47
1:A:1345:ARG:NE	1:A:1373:ASP:OD1	2.32	0.47
2:B:1081:LEU:O	3:C:189:THR:HG22	2.14	0.47
11:K:29:ASN:ND2	11:K:77:THR:OG1	2.48	0.47
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.97	0.46
2:B:810:GLU:HB3	2:B:815:ARG:CZ	2.45	0.46
1:A:100:LYS:HE3	1:A:174:ILE:O	2.16	0.46
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.80	0.46
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.97	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:HG	1.80	0.46
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.50	0.46
15:T:8:DT:H1'	15:T:9:DC:C5'	2.30	0.46
2:B:911:ILE:HG13	2:B:912:ILE:HG13	1.96	0.46
3:C:33:LEU:HG	3:C:37:MET:HE2	1.98	0.46
7:G:88:ASP:OD1	7:G:89:GLY:N	2.48	0.46
1:A:1341:ILE:HD11	1:A:1376:THR:HB	1.98	0.46
2:B:40:GLU:OE1	2:B:682:SER:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LEU:HB3	2:B:615:MET:SD	2.55	0.46
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.16	0.46
4:D:178:ALA:O	4:D:182:SER:N	2.46	0.46
9:I:73:ARG:HD2	9:I:101:PHE:CZ	2.51	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.97	0.46
2:B:271:ALA:HB2	2:B:282:ILE:HG22	1.97	0.46
2:B:848:ARG:HH22	2:B:996:ARG:HE	1.64	0.46
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.97	0.46
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.51	0.46
2:B:924:GLU:O	2:B:928:ARG:HB3	2.16	0.46
3:C:18:VAL:HG12	3:C:240:VAL:HG22	1.98	0.46
4:D:207:LEU:HG	4:D:211:LEU:HD13	1.98	0.46
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.98	0.45
2:B:821:GLN:OE1	2:B:851:PHE:N	2.45	0.45
15:T:8:DT:C1'	15:T:9:DC:H5'	2.32	0.45
1:A:152:VAL:HG23	1:A:162:VAL:HG23	1.97	0.45
2:B:37:PHE:HB2	2:B:681:TRP:CE3	2.51	0.45
4:D:58:VAL:HG13	7:G:49:LEU:HD11	1.98	0.45
1:A:120:GLU:HA	1:A:123:ARG:NH2	2.31	0.45
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.98	0.45
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.98	0.45
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.32	0.45
1:A:157:ASP:OD2	1:A:159:THR:OG1	2.35	0.45
2:B:874:PHE:O	12:L:42:ARG:NH1	2.39	0.45
3:C:84:ARG:HD3	11:K:11:LEU:HD11	1.98	0.45
7:G:15:PRO:HA	7:G:18:PHE:CD2	2.51	0.45
4:D:164:ILE:O	4:D:168:LYS:N	2.46	0.45
15:T:5:DC:H1'	15:T:6:DT:H5'	1.99	0.45
1:A:89:PRO:O	1:A:204:THR:OG1	2.29	0.45
1:A:338:GLY:C	2:B:1129:ARG:HH12	2.24	0.45
1:A:1392:SER:O	1:A:1394:THR:HG23	2.17	0.45
2:B:644:GLU:OE1	2:B:644:GLU:N	2.45	0.45
2:B:883:LEU:HD21	2:B:928:ARG:HD3	1.98	0.45
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.97	0.45
4:D:156:ASP:H	4:D:159:THR:HG22	1.81	0.45
1:A:1288:ASP:OD2	1:A:1300:LYS:HB3	2.16	0.45
2:B:886:LYS:HD2	2:B:940:PRO:HG3	1.98	0.45
2:B:1162:ILE:HG22	2:B:1169:MET:HA	1.99	0.45
4:D:31:GLN:N	4:D:31:GLN:OE1	2.49	0.45
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:HD3	1:A:645:LEU:HD13	1.99	0.45
15:T:19:DC:H2'	15:T:20:DT:C6	2.52	0.45
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.52	0.44
2:B:166:PHE:CZ	2:B:169:ARG:HG3	2.52	0.44
2:B:428:ILE:HD11	2:B:448:ILE:HA	1.99	0.44
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.51	0.44
9:I:29:CYS:HB2	9:I:34:TYR:HB3	1.99	0.44
11:K:102:LYS:NZ	11:K:106:GLU:OE2	2.38	0.44
1:A:905:ASP:OD1	1:A:905:ASP:N	2.50	0.44
1:A:1196:GLU:N	1:A:1196:GLU:OE1	2.50	0.44
2:B:760:ASP:OD1	2:B:760:ASP:N	2.48	0.44
4:D:165:GLN:HA	4:D:168:LYS:HB3	1.99	0.44
4:D:208:GLU:O	4:D:212:LYS:HG2	2.17	0.44
1:A:92:HIS:HD2	1:A:94:GLY:H	1.66	0.44
1:A:885:THR:HG23	1:A:1024:SER:HB2	2.00	0.44
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.00	0.44
2:B:335:GLY:HA3	2:B:348:ARG:HB3	1.97	0.44
2:B:841:MET:HE3	2:B:1010:LEU:HD21	1.99	0.44
3:C:10:ILE:HG22	3:C:20:PHE:HB3	1.98	0.44
1:A:451:HIS:ND1	1:A:453:MET:HB2	2.32	0.44
7:G:109:PHE:O	7:G:160:ILE:HA	2.17	0.44
7:G:118:ASP:OD1	7:G:119:LEU:N	2.51	0.44
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.00	0.44
2:B:883:LEU:HG	2:B:932:HIS:HB3	1.98	0.44
4:D:25:ALA:H	7:G:84:GLY:HA3	1.82	0.44
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.00	0.44
7:G:88:ASP:HA	7:G:144:ARG:HA	1.99	0.44
10:J:44:TYR:HA	10:J:47:ARG:HB2	2.00	0.44
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.99	0.44
1:A:557:ASP:N	1:A:557:ASP:OD1	2.48	0.44
4:D:33:PHE:HD1	4:D:47:LEU:HD21	1.83	0.44
4:D:67:ARG:HH21	4:D:68:ARG:NH1	2.15	0.44
6:F:85:MET:HE1	6:F:148:VAL:HG13	2.00	0.44
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.52	0.44
11:K:53:ASP:OD1	11:K:54:ARG:N	2.50	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.51	0.44
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.53	0.43
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.00	0.43
3:C:21:ILE:HG12	3:C:229:TYR:CD2	2.53	0.43
8:H:123:MET:HE2	8:H:142:LEU:HD13	2.00	0.43
1:A:99:ILE:HD11	1:A:234:MET:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:617:ARG:NH2	9:I:61:ASP:OD2	2.50	0.43
9:I:113:ASP:HB3	9:I:116:ASN:HB3	2.00	0.43
11:K:30:ALA:HB2	11:K:76:GLN:HG3	2.01	0.43
1:A:608:ILE:HD12	1:A:613:ILE:HG13	2.01	0.43
1:A:881:GLN:CD	1:A:959:ASN:HA	2.44	0.43
1:A:922:ASP:OD1	1:A:923:LEU:N	2.51	0.43
4:D:23:ASN:H	4:D:28:GLN:HB2	1.83	0.43
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.19	0.43
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.19	0.43
2:B:910:VAL:HA	2:B:940:PRO:HA	2.00	0.43
6:F:116:ASP:HB3	6:F:119:ARG:HG2	2.00	0.43
8:H:125:LEU:HD23	8:H:135:LEU:HD11	2.00	0.43
2:B:315:LYS:HB3	9:I:4:PHE:CZ	2.54	0.43
2:B:863:GLU:HG2	2:B:962:LYS:O	2.18	0.43
4:D:48:ILE:HG13	4:D:48:ILE:O	2.19	0.43
13:N:5:DG:N2	13:N:7:DG:N3	2.65	0.43
14:P:1:G:H2'	14:P:2:G:C8	2.54	0.43
1:A:786:HIS:HE1	2:B:519:TRP:NE1	2.17	0.43
2:B:232:SER:O	2:B:261:ARG:NH1	2.42	0.43
2:B:629:ASP:OD1	2:B:629:ASP:N	2.52	0.43
3:C:22:LEU:HG	3:C:25:VAL:HG11	2.00	0.43
9:I:22:ASN:HB2	9:I:24:ARG:HH11	1.83	0.43
1:A:148:CYS:HB3	1:A:168:GLY:H	1.84	0.43
1:A:1173:HIS:CE1	1:A:1229:SER:HA	2.53	0.43
3:C:46:ILE:HA	3:C:159:ALA:HA	2.01	0.43
7:G:63:PRO:C	7:G:65:ASP:H	2.27	0.43
1:A:105:CYS:SG	1:A:139:TRP:HA	2.58	0.43
1:A:447:GLN:HG2	2:B:1134:GLU:OE2	2.19	0.43
1:A:1148:ILE:N	1:A:1196:GLU:O	2.47	0.43
2:B:773:MET:HE1	2:B:987:LYS:HB3	2.00	0.43
4:D:66:ARG:HG2	7:G:51:TYR:CG	2.53	0.43
5:E:118:PRO:HA	5:E:121:MET:HB2	2.01	0.43
6:F:127:GLU:HG3	6:F:129:LYS:HG2	2.00	0.43
2:B:244:LEU:HD23	2:B:244:LEU:H	1.83	0.43
4:D:172:LEU:HG	4:D:173:HIS:H	1.84	0.43
9:I:111:THR:HG23	9:I:113:ASP:H	1.82	0.43
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.50	0.43
3:C:55:THR:HG1	3:C:152:GLU:H	1.61	0.43
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.84	0.42
1:A:338:GLY:O	2:B:1129:ARG:NH1	2.46	0.42
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:HA3	1:A:469:ARG:HB2	2.00	0.42
1:A:918:GLU:N	1:A:918:GLU:OE1	2.52	0.42
1:A:1227:ILE:HG13	1:A:1239:ARG:HB2	2.01	0.42
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.84	0.42
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.19	0.42
1:A:1403:GLU:CD	15:T:17:DT:H4'	2.44	0.42
2:B:868:MET:N	2:B:868:MET:SD	2.92	0.42
8:H:118:PHE:HZ	8:H:123:MET:HE3	1.84	0.42
2:B:175:ARG:HG3	2:B:200:GLY:HA3	2.00	0.42
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.42
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.02	0.42
1:A:754:SER:OG	1:A:755:PHE:N	2.53	0.42
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.52	0.42
4:D:177:VAL:O	4:D:181:GLY:N	2.45	0.42
10:J:21:TYR:O	10:J:25:LEU:HD23	2.19	0.42
2:B:59:LEU:HD11	2:B:170:LEU:HD22	2.01	0.42
2:B:133:LYS:HD3	2:B:135:ARG:HE	1.85	0.42
2:B:433:GLN:HA	2:B:436:VAL:HG12	2.02	0.42
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.20	0.42
2:B:862:GLN:HA	2:B:963:PHE:HB2	2.00	0.42
2:B:365:THR:HG21	2:B:370:PHE:HB2	2.02	0.42
2:B:981:ALA:HB2	2:B:987:LYS:HA	2.01	0.42
4:D:195:ILE:HD12	4:D:198:LEU:HD11	2.00	0.42
7:G:165:GLU:O	7:G:168:LEU:HB2	2.20	0.42
8:H:63:LEU:O	8:H:89:LEU:N	2.41	0.42
8:H:104:PHE:CE1	8:H:137:GLN:HG2	2.55	0.42
1:A:119:ASN:OD1	1:A:120:GLU:N	2.53	0.42
1:A:1403:GLU:HG2	15:T:17:DT:H5''	2.02	0.42
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.54	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.55	0.42
2:B:230:ALA:HA	2:B:261:ARG:NH2	2.34	0.42
7:G:44:TYR:CD2	7:G:105:PRO:HG2	2.54	0.42
1:A:698:GLN:O	9:I:112:SER:OG	2.33	0.42
1:A:783:THR:O	2:B:516:ASN:HB3	2.20	0.42
3:C:145:CYS:SG	3:C:146:LYS:N	2.93	0.42
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.55	0.42
5:E:79:TRP:CD1	5:E:96:PHE:HE1	2.36	0.42
1:A:114:LEU:HD23	1:A:145:LYS:HG3	2.02	0.42
1:A:182:VAL:HG12	1:A:201:VAL:HG22	2.02	0.42
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.55	0.42
1:A:1220:PHE:HD2	1:A:1224:LEU:HD22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.52	0.42
2:B:415:GLN:HE21	2:B:466:TRP:CD1	2.38	0.42
2:B:421:PHE:HA	2:B:453:ILE:HD11	2.01	0.42
2:B:554:ILE:HD11	2:B:613:VAL:HG21	2.01	0.42
2:B:691:GLU:OE1	2:B:740:HIS:NE2	2.38	0.42
2:B:903:VAL:O	2:B:949:VAL:HG12	2.19	0.42
4:D:40:HIS:CE1	7:G:6:ASP:HB3	2.54	0.42
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.51	0.41
1:A:1197:LEU:HD12	1:A:1209:MET:SD	2.60	0.41
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.03	0.41
1:A:1252:THR:O	1:A:1256:GLU:N	2.54	0.41
1:A:1378:GLN:OE1	5:E:177:ARG:NH1	2.53	0.41
7:G:93:SER:O	7:G:99:PHE:HB2	2.21	0.41
8:H:2:SER:N	8:H:61:SER:HG	2.18	0.41
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.20	0.41
1:A:889:SER:O	1:A:893:PHE:N	2.41	0.41
2:B:643:ASP:OD2	2:B:654:ARG:NH2	2.53	0.41
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.85	0.41
3:C:90:ASP:OD1	3:C:91:HIS:N	2.52	0.41
4:D:188:ALA:HA	4:D:207:LEU:HD22	2.02	0.41
8:H:7:ASP:OD1	8:H:7:ASP:N	2.51	0.41
10:J:58:GLU:O	10:J:62:ARG:HG2	2.20	0.41
1:A:92:HIS:CD2	1:A:94:GLY:H	2.38	0.41
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.53	0.41
1:A:779:PHE:CZ	2:B:517:THR:HA	2.55	0.41
1:A:1031:VAL:HG13	1:A:1037:LEU:HB2	2.02	0.41
2:B:343:ILE:HB	2:B:348:ARG:HE	1.85	0.41
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.53	0.41
1:A:349:ALA:HB2	1:A:374:LEU:HD11	2.02	0.41
1:A:867:ILE:HG22	5:E:208:TYR:HE1	1.86	0.41
2:B:762:ASN:HD21	2:B:984:HIS:HB3	1.85	0.41
3:C:148:ARG:N	3:C:151:GLN:OE1	2.38	0.41
7:G:13:LEU:HD11	7:G:26:LEU:HG	2.02	0.41
1:A:22:PHE:HE2	2:B:1208:MET:HA	1.86	0.41
1:A:853:ASP:OD1	1:A:855:THR:OG1	2.30	0.41
1:A:1158:PRO:HG2	1:A:1185:PHE:HB3	2.03	0.41
1:A:1261:LYS:O	1:A:1265:ASN:N	2.48	0.41
2:B:195:CYS:SG	2:B:783:THR:OG1	2.49	0.41
2:B:616:ILE:O	2:B:624:LEU:HD12	2.20	0.41
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.03	0.41
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:HD12	9:I:6:PHE:HZ	1.84	0.41
2:B:355:ILE:HD13	2:B:359:GLU:HG3	2.01	0.41
2:B:839:MET:HE2	2:B:1010:LEU:HD22	2.01	0.41
2:B:1217:TYR:CE2	4:D:13:ARG:HD3	2.56	0.41
3:C:10:ILE:HG23	11:K:108:GLU:HG2	2.01	0.41
1:A:259:GLU:HB2	1:A:264:PHE:CE2	2.55	0.41
1:A:515:GLN:HE21	1:A:1363:VAL:HG22	1.84	0.41
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.53	0.41
4:D:69:ALA:HA	4:D:72:ARG:HG2	2.03	0.41
5:E:118:PRO:O	5:E:122:LYS:HG2	2.21	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
1:A:527:THR:HG21	1:A:650:GLN:HA	2.03	0.41
1:A:1394:THR:H	1:A:1399:ARG:HD3	1.85	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.03	0.41
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.21	0.41
2:B:1129:ARG:HB3	15:T:21:DT:O3'	2.21	0.41
2:B:1152:MET:HE3	2:B:1152:MET:HB3	1.97	0.41
5:E:96:PHE:CE2	5:E:132:ILE:HD12	2.56	0.41
6:F:133:VAL:HG12	6:F:147:SER:HA	2.03	0.41
7:G:81:PRO:HB3	7:G:106:MET:SD	2.61	0.41
9:I:77:LYS:HD3	9:I:108:HIS:CD2	2.55	0.41
13:N:9:DG:H1	15:T:10:DC:H42	1.68	0.41
1:A:875:ALA:HB1	1:A:1364:ASN:HD22	1.86	0.41
1:A:1004:ASN:OD1	1:A:1007:ILE:HG12	2.21	0.41
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.36	0.41
2:B:778:MET:HE3	2:B:778:MET:HB2	1.94	0.41
3:C:258:ILE:CG1	11:K:42:LEU:HD21	2.48	0.40
8:H:36:CYS:HA	8:H:126:GLU:O	2.20	0.40
1:A:64:ASN:ND2	2:B:924:GLU:HB2	2.35	0.40
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.52	0.40
1:A:571:LEU:HD12	8:H:46:LEU:HD22	2.01	0.40
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	2.04	0.40
1:A:1424:VAL:HG22	1:A:1436:ILE:HG21	2.03	0.40
1:A:786:HIS:HE1	2:B:519:TRP:CE2	2.39	0.40
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.21	0.40
1:A:1252:THR:HA	1:A:1255:GLU:HG2	2.02	0.40
2:B:558:LEU:HD11	2:B:626:ILE:HD12	2.02	0.40
5:E:163:GLU:O	5:E:167:ARG:HG2	2.20	0.40
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	2.02	0.40
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	2.04	0.40
2:B:135:ARG:CD	2:B:155:GLU:HG3	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:LYS:HA	5:E:97:VAL:HG12	2.04	0.40
5:E:135:PHE:HZ	5:E:186:LEU:O	2.04	0.40
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.56	0.40
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.04	0.40
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.61	0.40
2:B:1001:PHE:CE2	3:C:178:PHE:HB3	2.57	0.40
4:D:63:LEU:HB3	4:D:129:LEU:HD21	2.04	0.40
7:G:4:ILE:HG22	7:G:77:VAL:HA	2.03	0.40
13:N:3:DG:H2''	13:N:4:DA:C8	2.56	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	1415/1733 (82%)	1371 (97%)	44 (3%)	0	100	100
2	B	1173/1224 (96%)	1130 (96%)	43 (4%)	0	100	100
3	C	263/318 (83%)	253 (96%)	10 (4%)	0	100	100
4	D	161/221 (73%)	158 (98%)	3 (2%)	0	100	100
5	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
6	F	85/155 (55%)	81 (95%)	4 (5%)	0	100	100
7	G	169/171 (99%)	160 (95%)	9 (5%)	0	100	100
8	H	135/146 (92%)	130 (96%)	5 (4%)	0	100	100
9	I	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
All	All	3950/4565 (86%)	3819 (97%)	131 (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	1245/1520 (82%)	1245 (100%)	0	100	100
2	B	1026/1061 (97%)	1026 (100%)	0	100	100
3	C	233/274 (85%)	233 (100%)	0	100	100
4	D	147/200 (74%)	147 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	122/128 (95%)	122 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3511/4009 (88%)	3511 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	92	HIS
1	A	118	HIS
1	A	171	GLN
1	A	253	ASN
1	A	256	GLN
1	A	479	ASN
1	A	515	GLN
1	A	786	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	862	ASN
1	A	877	HIS
1	A	903	ASN
1	A	975	HIS
1	A	1048	ASN
1	A	1070	GLN
1	A	1078	GLN
1	A	1265	ASN
2	B	121	ASN
2	B	357	GLN
2	B	383	ASN
2	B	465	ASN
2	B	513	GLN
2	B	706	GLN
2	B	762	ASN
2	B	843	GLN
2	B	984	HIS
2	B	1076	HIS
3	C	195	GLN
5	E	115	ASN
8	H	35	GLN
9	I	90	GLN
9	I	108	HIS
10	J	53	HIS
11	K	29	ASN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	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, 9 are monoatomic - leaving 1 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	$\# Z > 2$
18	CPT	T	101	15,13	0,2,4	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

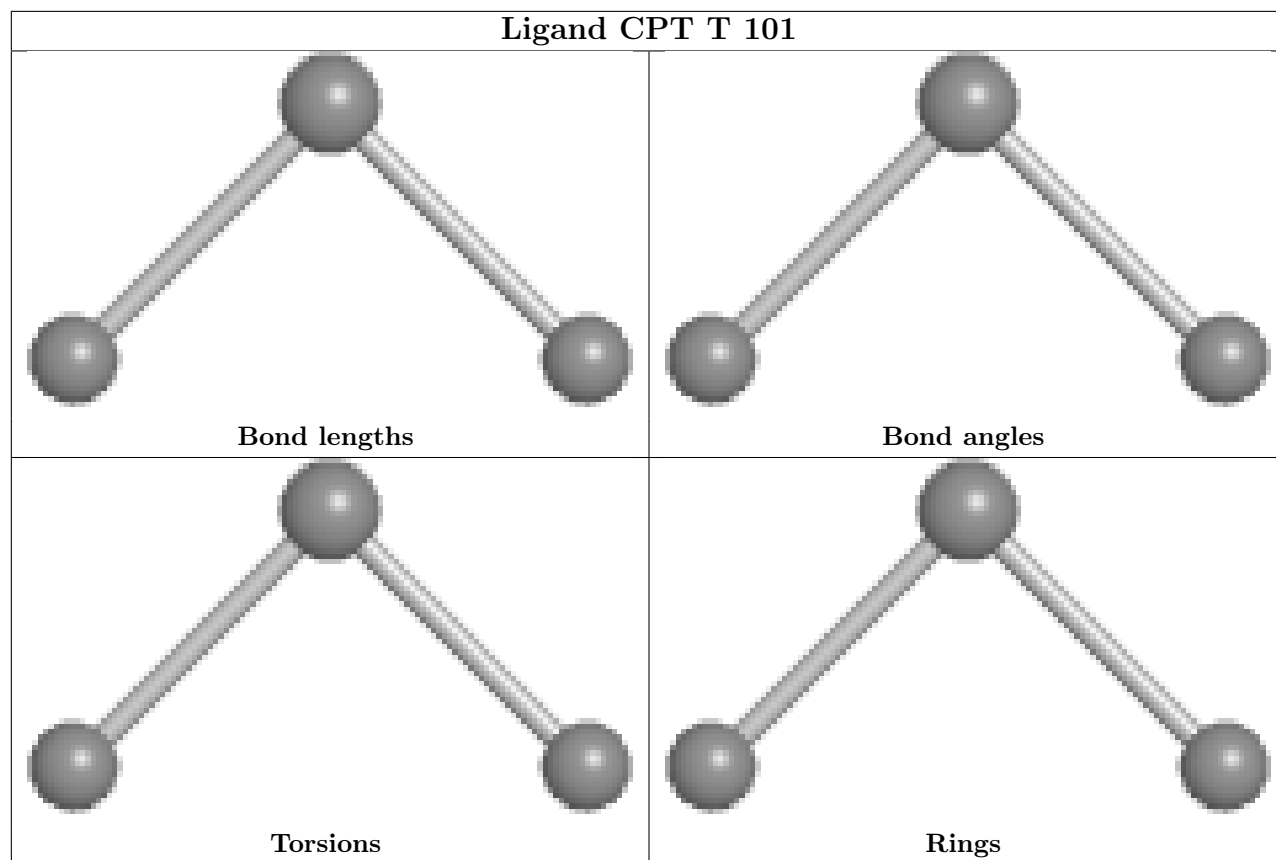
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

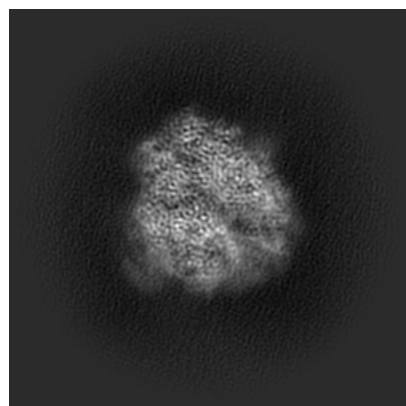
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66162. These allow visual inspection of the internal detail of the map and identification of artifacts.

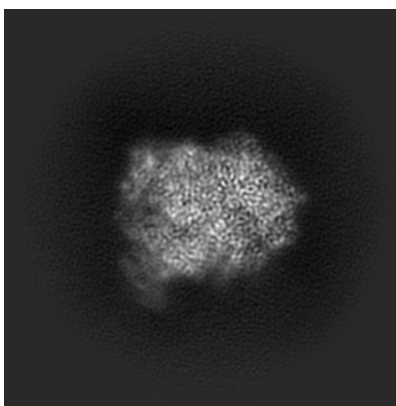
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

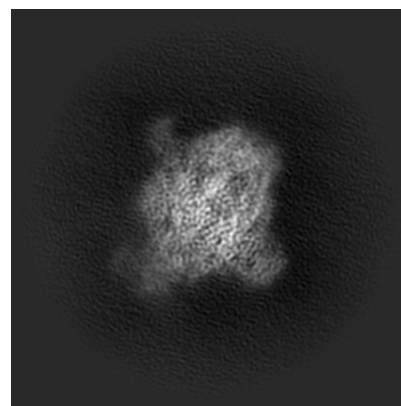
6.1.1 Primary map



X

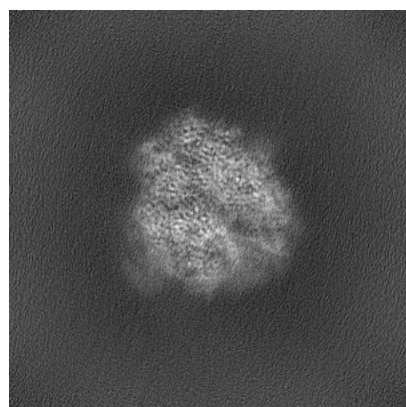


Y

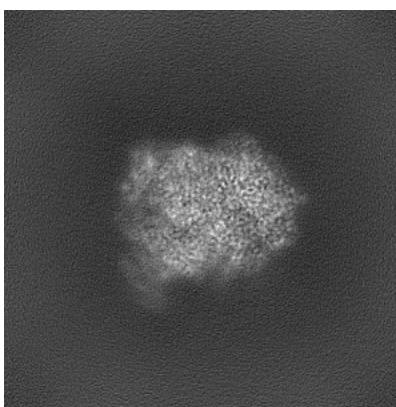


Z

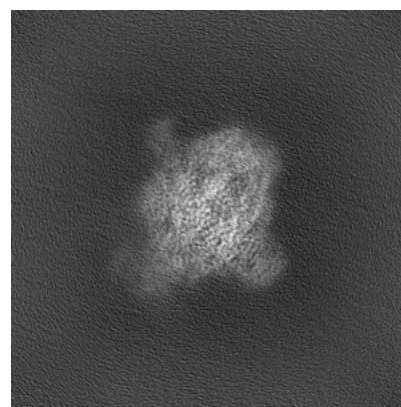
6.1.2 Raw map



X



Y

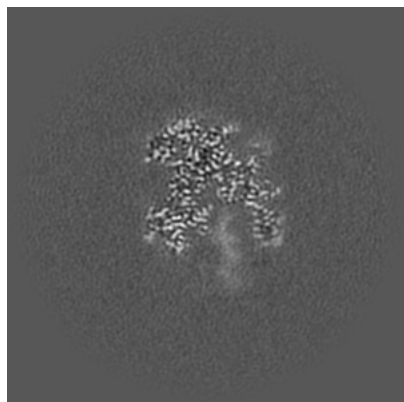


Z

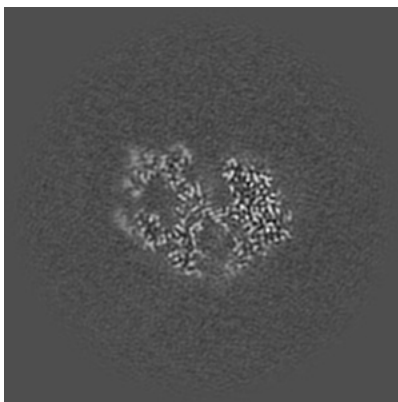
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

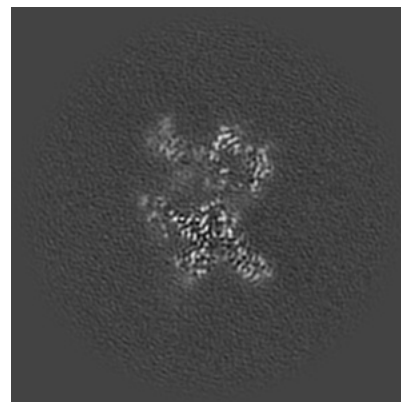
6.2.1 Primary map



X Index: 160

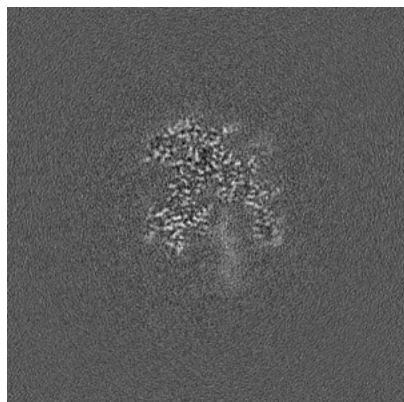


Y Index: 160

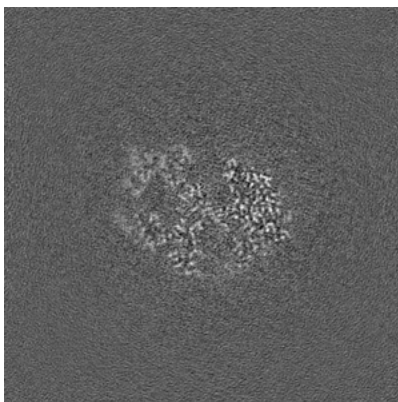


Z Index: 160

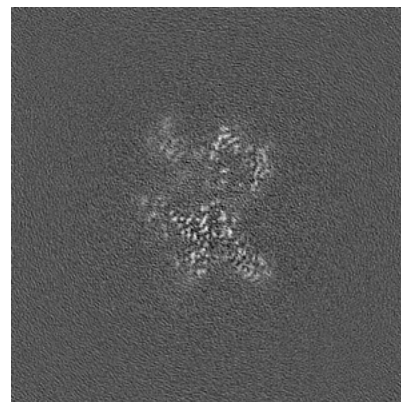
6.2.2 Raw map



X Index: 160



Y Index: 160

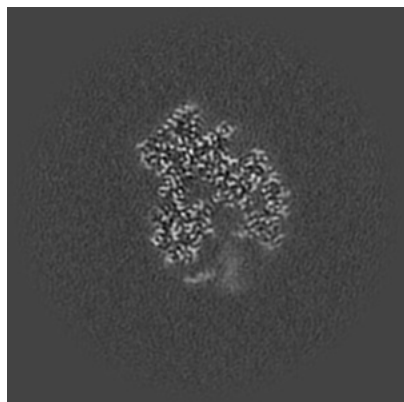


Z Index: 160

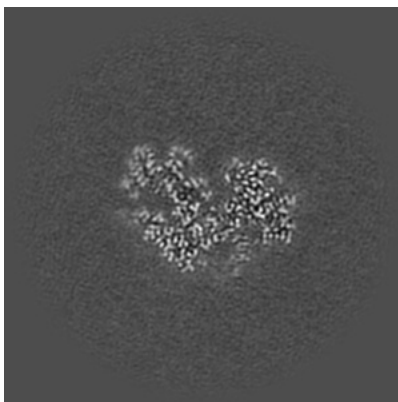
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

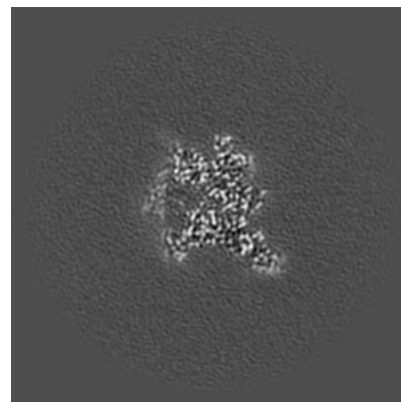
6.3.1 Primary map



X Index: 169

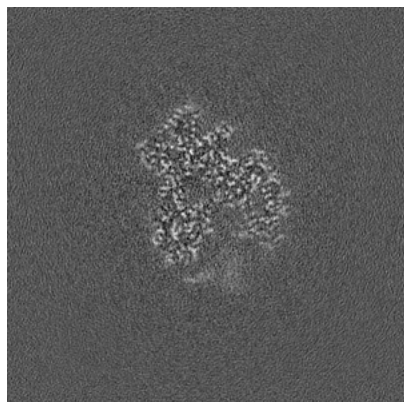


Y Index: 154

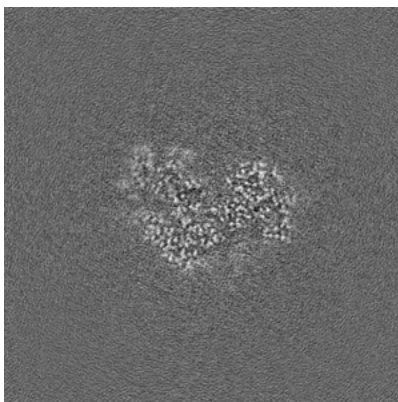


Z Index: 182

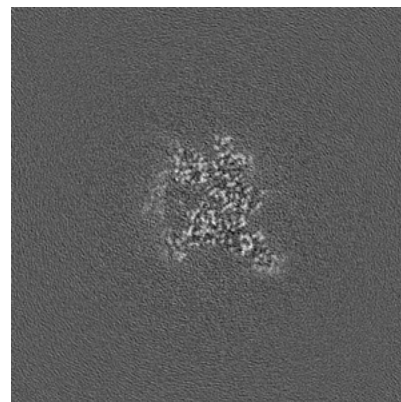
6.3.2 Raw map



X Index: 169



Y Index: 153

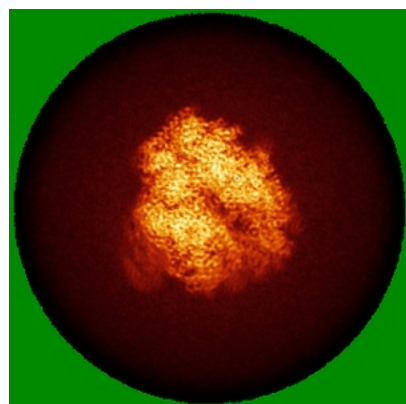


Z Index: 182

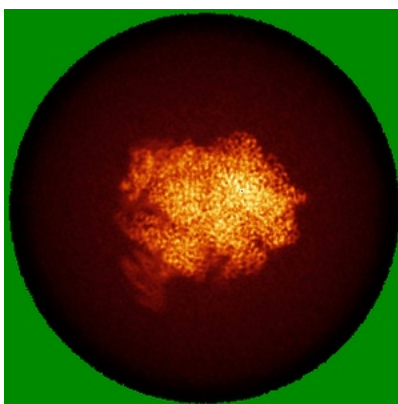
The images above show the largest variance slices of the map in three orthogonal directions.

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

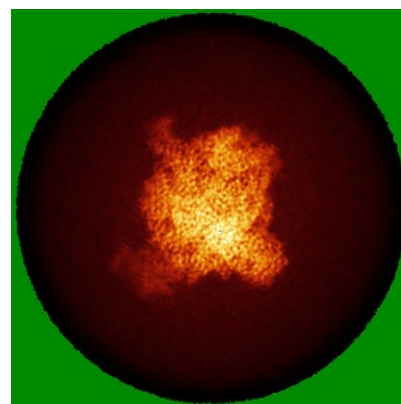
6.4.1 Primary map



X

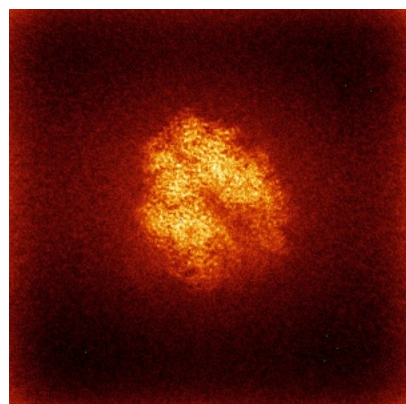


Y

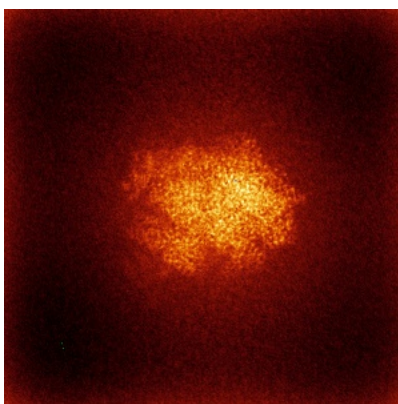


Z

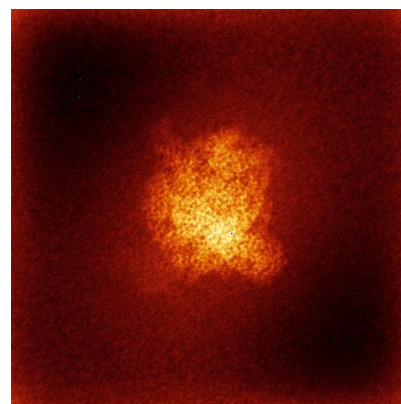
6.4.2 Raw map



X



Y

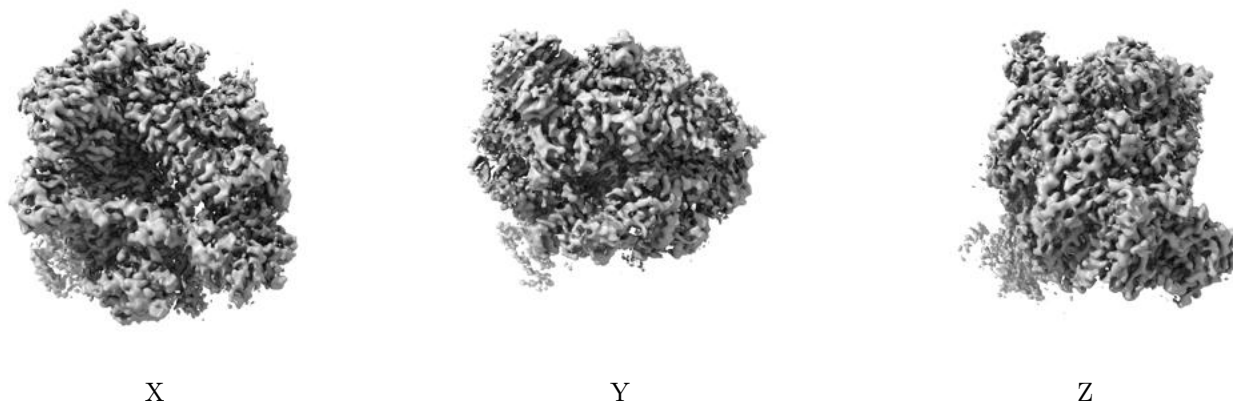


Z

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.

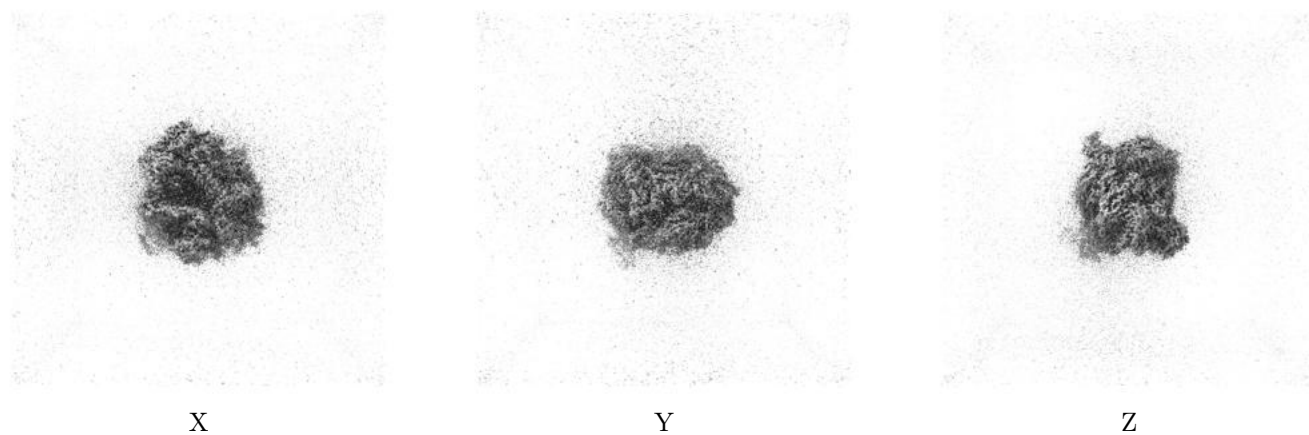
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

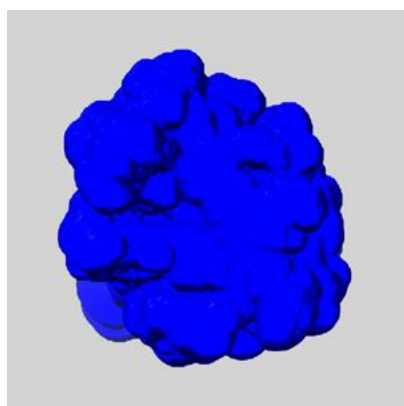
6.6 Mask visualisation [i](#)

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

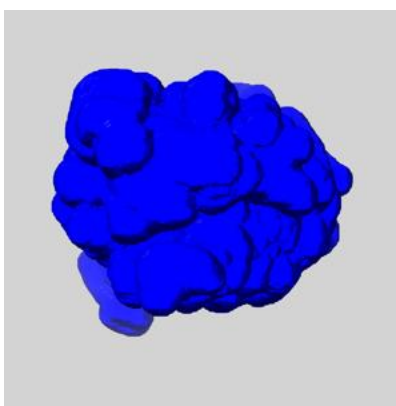
A mask typically either:

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

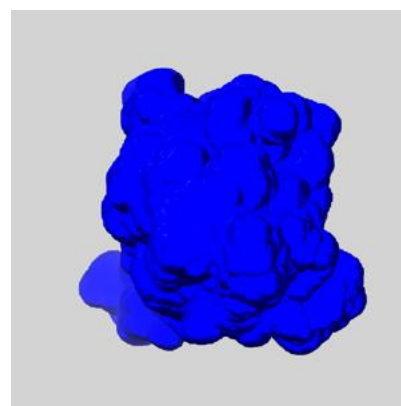
6.6.1 emd_66162_msk_1.map [i](#)



X



Y

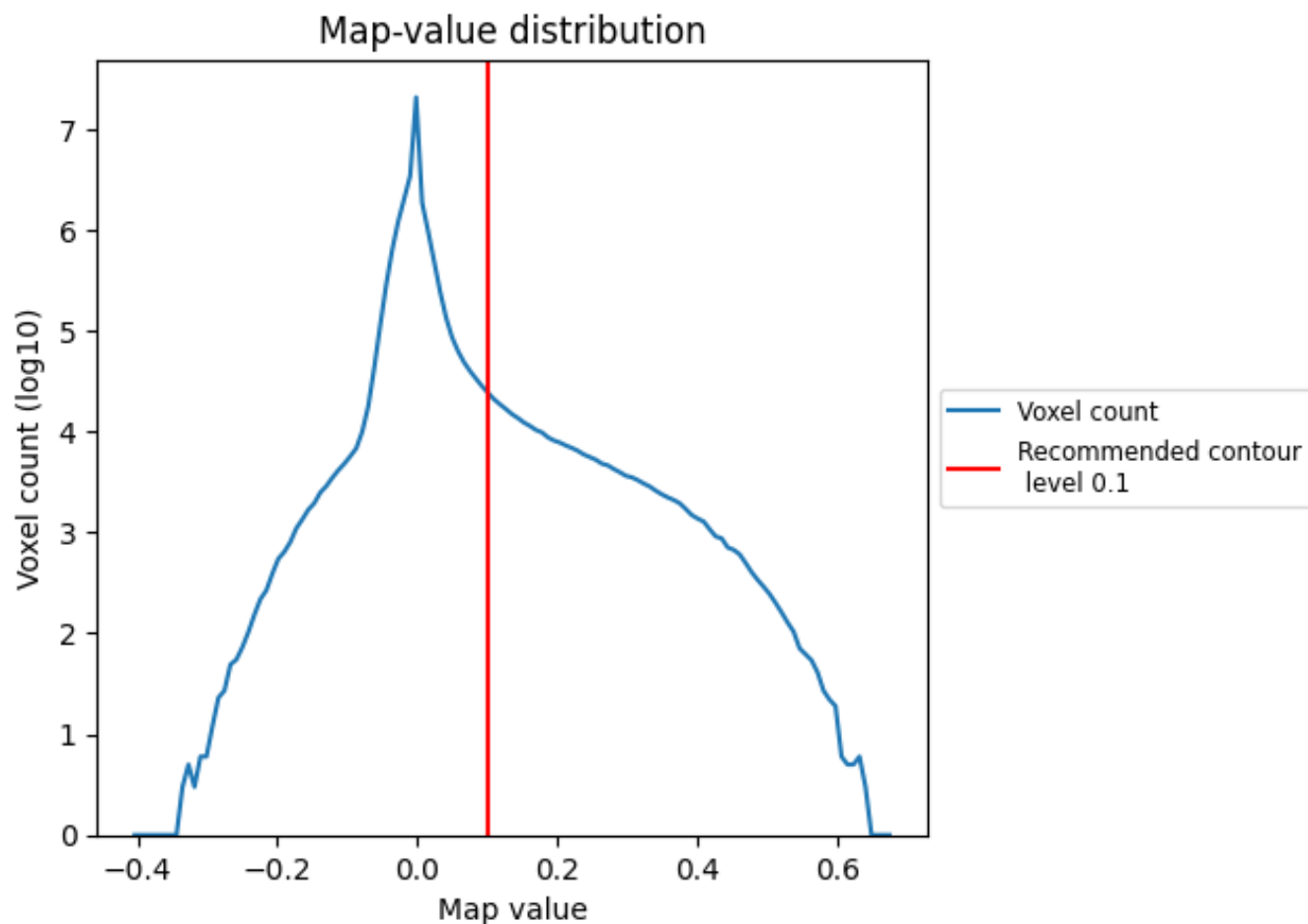


Z

7 Map analysis [i](#)

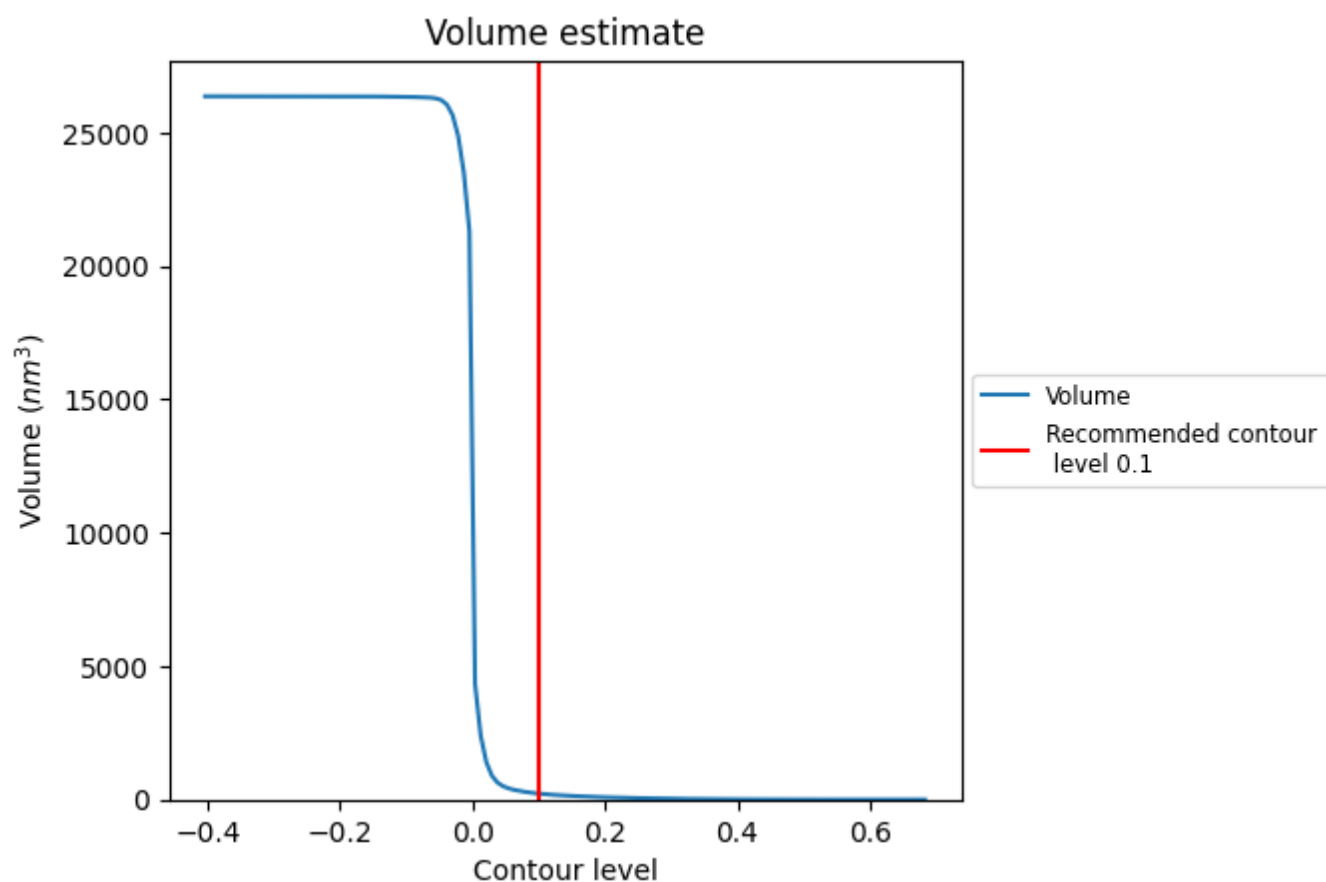
This section contains the results of statistical analysis of the map.

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.

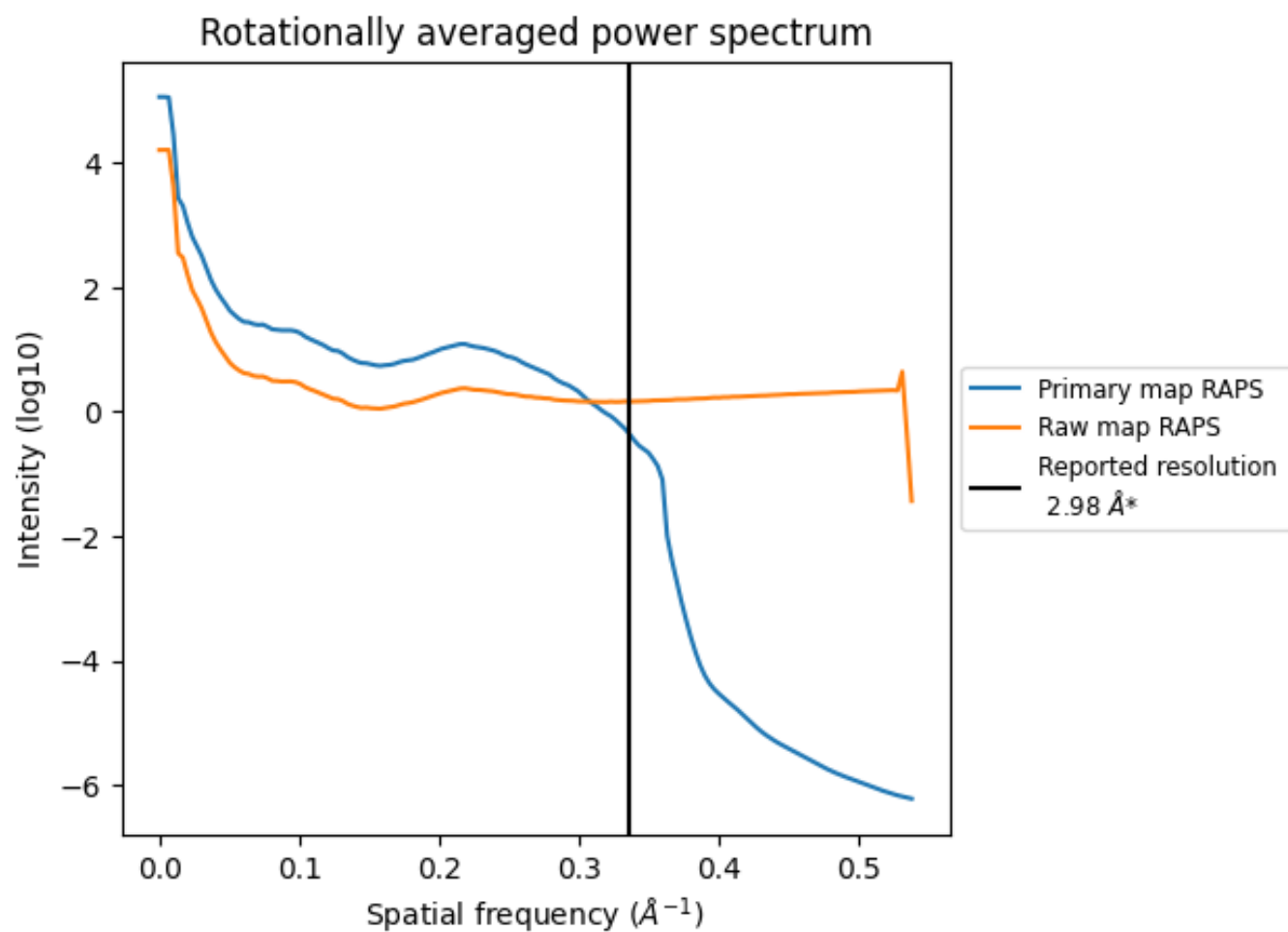
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 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 ⓘ

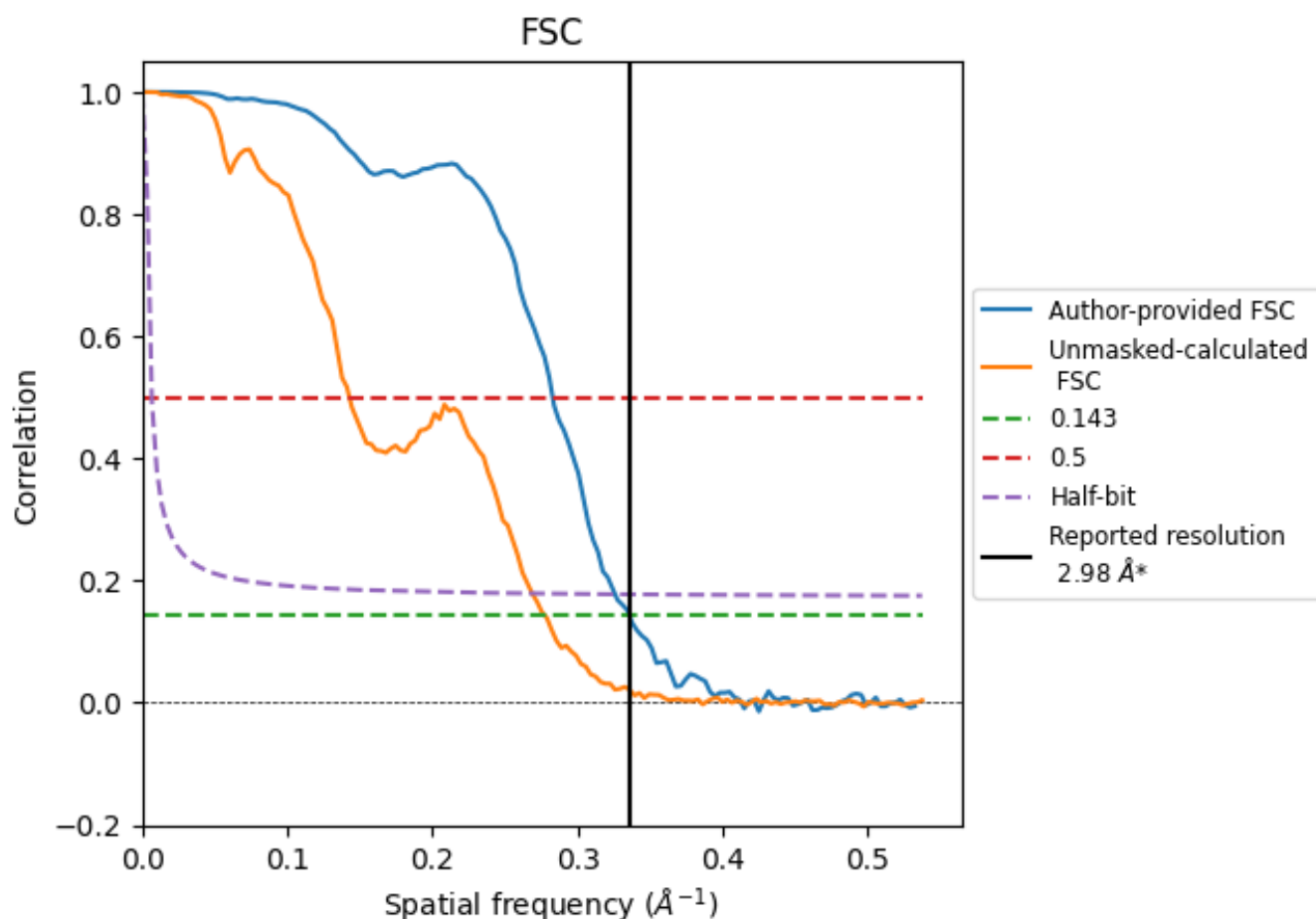


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

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 0.336 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

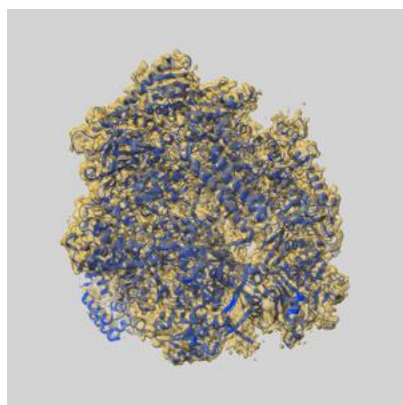
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.53	3.07
Unmasked-calculated*	3.60	7.00	3.72

*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 3.60 differs from the reported value 2.98 by more than 10 %

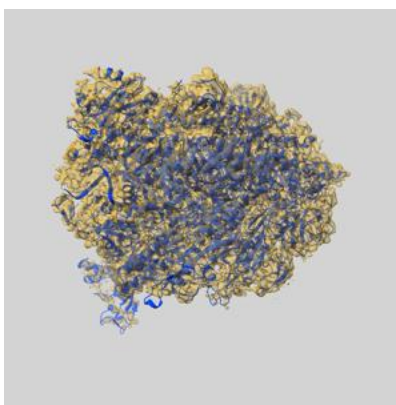
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66162 and PDB model 9WQ8. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

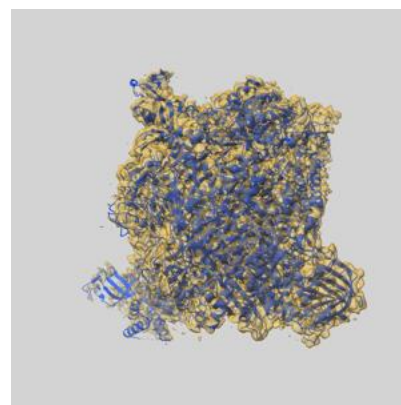
9.1 Map-model overlay [i](#)



X



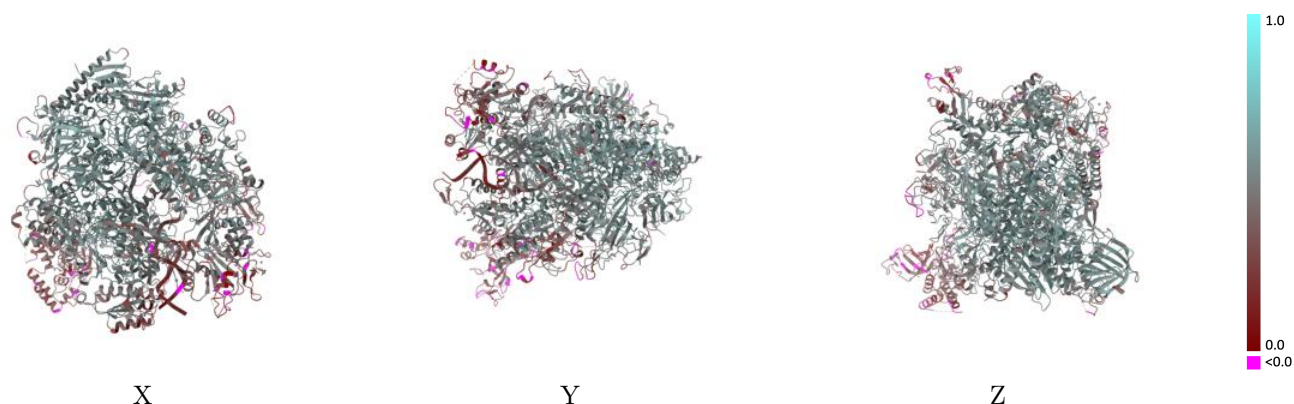
Y



Z

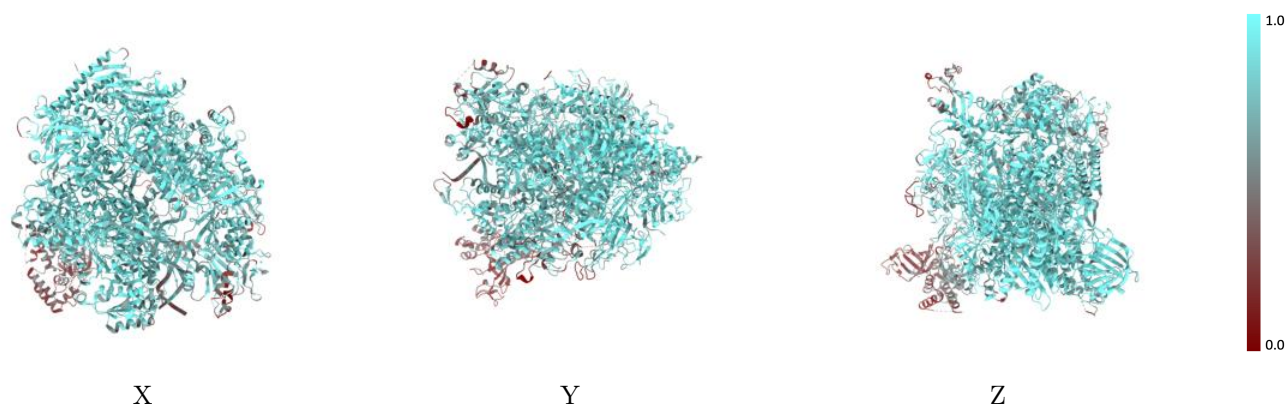
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



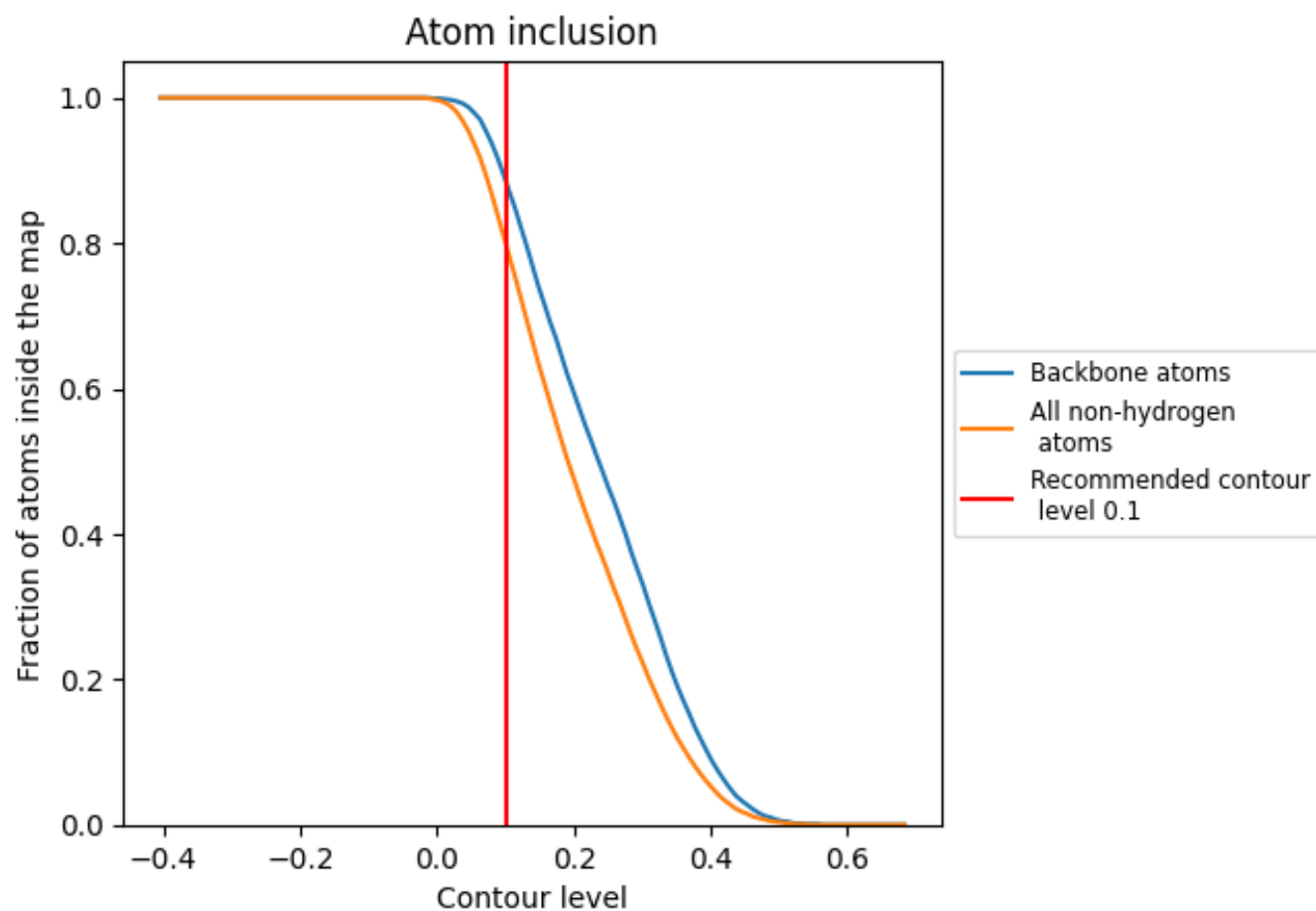
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4690
A	 0.8490	 0.4990
B	 0.8370	 0.4940
C	 0.8850	 0.5290
D	 0.2870	 0.1850
E	 0.8280	 0.4510
F	 0.8840	 0.5250
G	 0.4020	 0.2620
H	 0.8390	 0.5040
I	 0.7490	 0.4000
J	 0.8950	 0.5360
K	 0.8890	 0.5420
L	 0.8440	 0.4530
N	 0.6670	 0.2020
P	 0.9260	 0.5140
T	 0.7180	 0.3590

