



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:35 PM UTC

PDB ID : 8S54 / pdb_00008s54
EMDB ID : EMD-19720
Title : RNA polymerase II early elongation complex bound to TFIIE and TFIIF - state b (composite structure)
Authors : Zhan, Y.; Grabber, F.; Oberbeckmann, E.; Dienemann, C.; Cramer, P.
Deposited on : 2024-02-22
Resolution : 3.40 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:

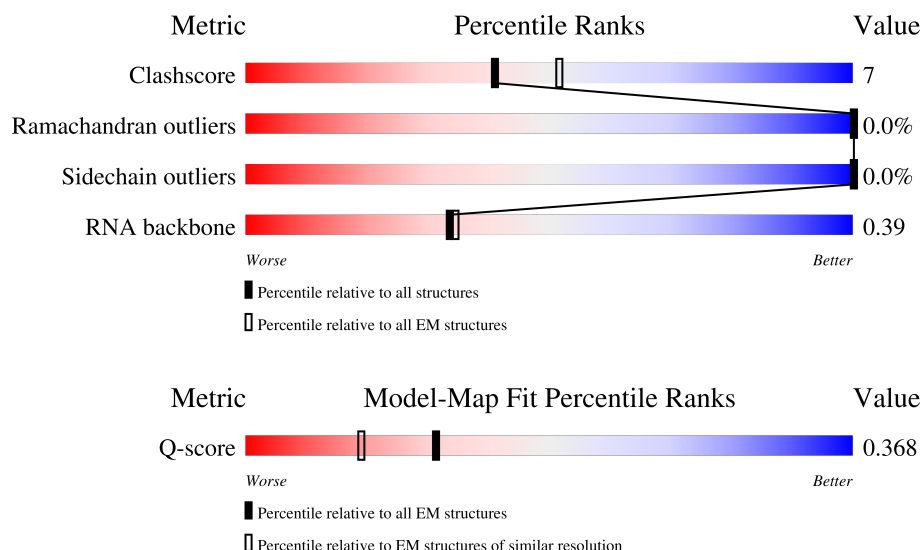
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



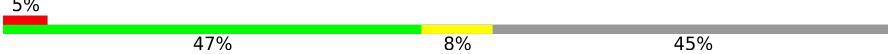
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1984	
2	B	1300	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	139	
14	P	14	
15	Q	517	
16	R	249	
17	T	139	
18	W	439	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 36745 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1417	Total	C	N	O	S	0	0
			11234	7070	2010	2082	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1130	Total	C	N	O	S	0	0
			9030	5714	1587	1665	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- 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
			1351	875	219	249	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	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	114	Total	C	N	O	S	0	0
			916	591	151	172	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	35	Total	C	N	O	P	0	0
			712	339	132	207	34		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	14	Total	C	N	O	P	0	0
			296	133	56	93	14		

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	137	Total	C	N	O	S	0	0
			1070	666	193	209	2		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	46	Total	C	N	O	P	0	0
			949	449	175	279	46		

- Molecule 18 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms		AltConf
19	W	1	Total	Zn	0
			1	1	

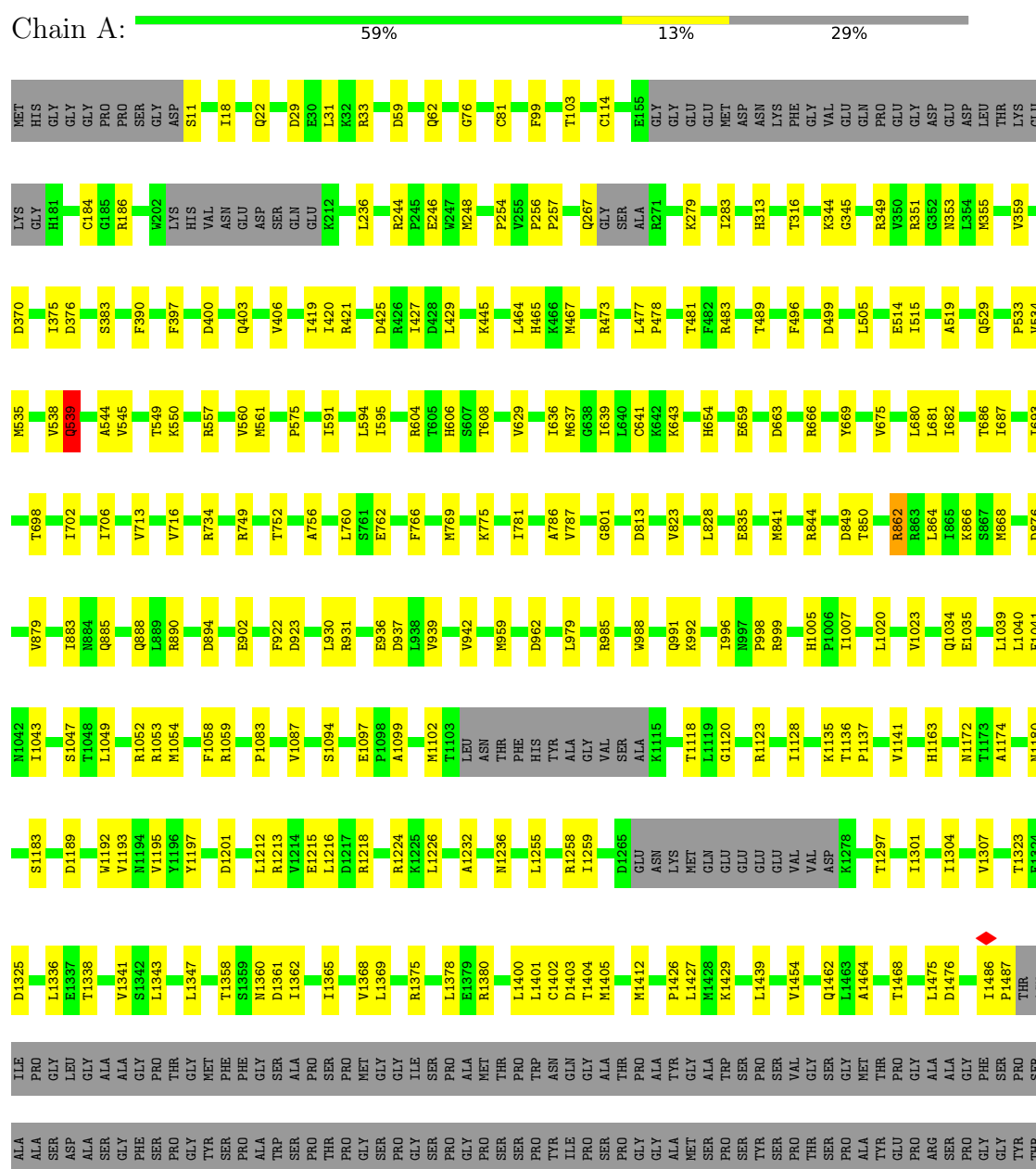
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	P	1	Total	Mg	0
			1	1	

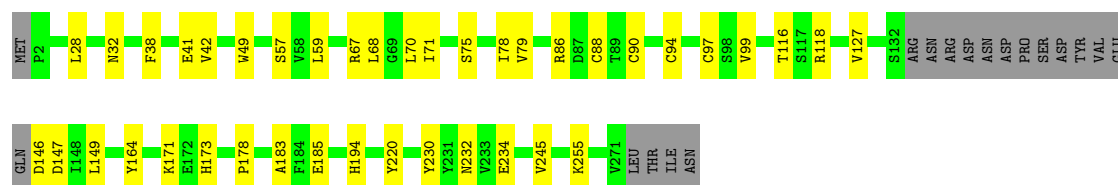
3 Residue-property plots

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 subunit

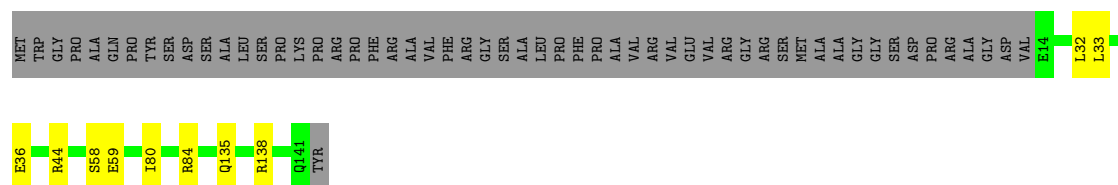


Chain C:  79% 15% 7%



• Molecule 4: RNA polymerase II subunit D

Chain D:  64% 5% 30%



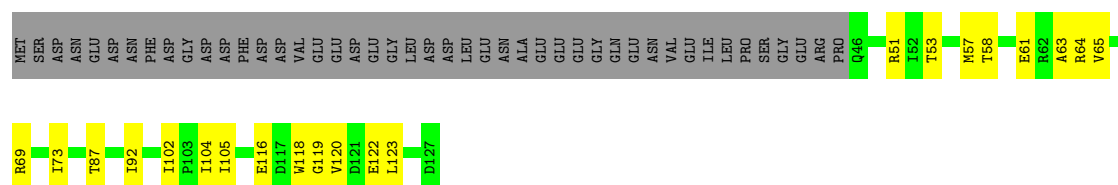
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  85% 14%



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

Chain F:  48% 17% 35%



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

Chain G:  87% 12%

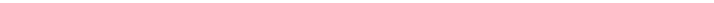


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  78% 21%



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

Chain I:  72% 19% 9%

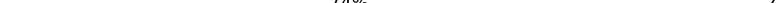


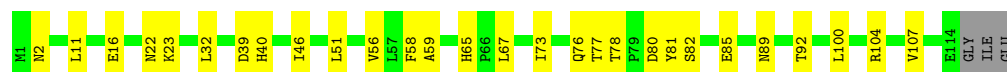
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  75% 25%

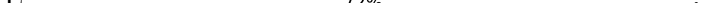


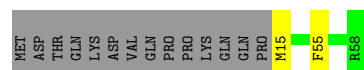
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  74% 24%



- Molecule 12: RNA polymerase II subunit K

Chain L:  72% 24%



- Molecule 13: Non-template DNA

Chain N: 22% . 75%

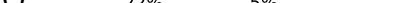


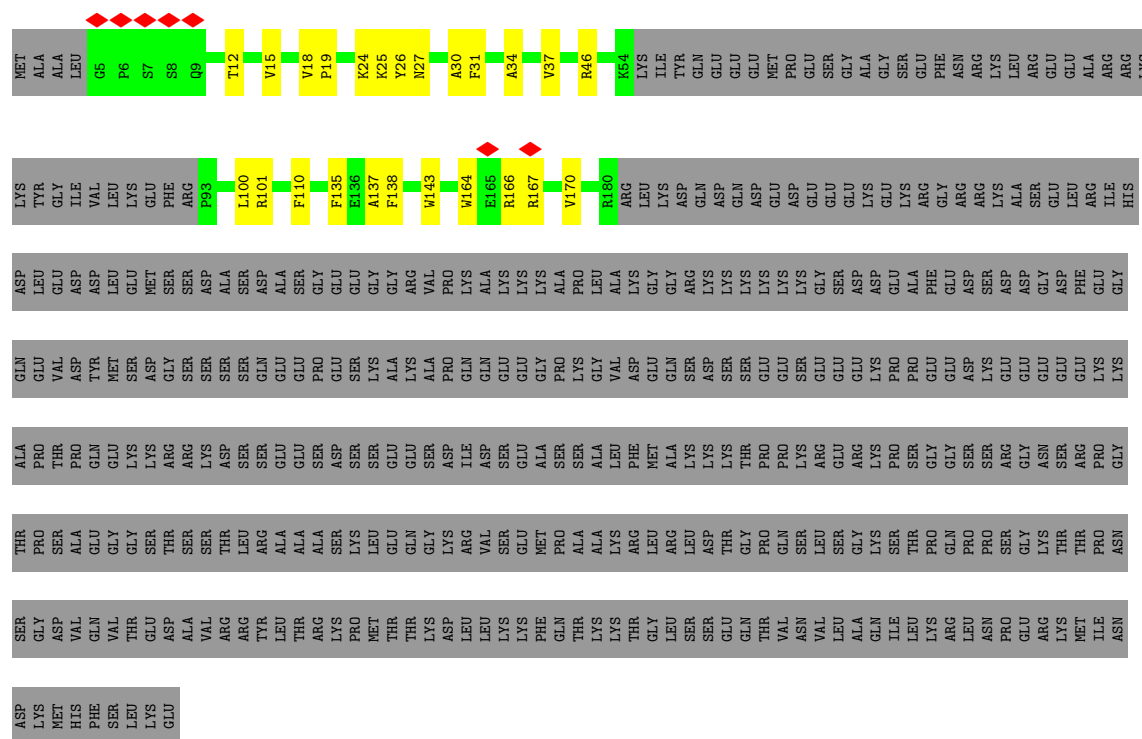
- Molecule 14: RNA

Chain P: 71% 29%

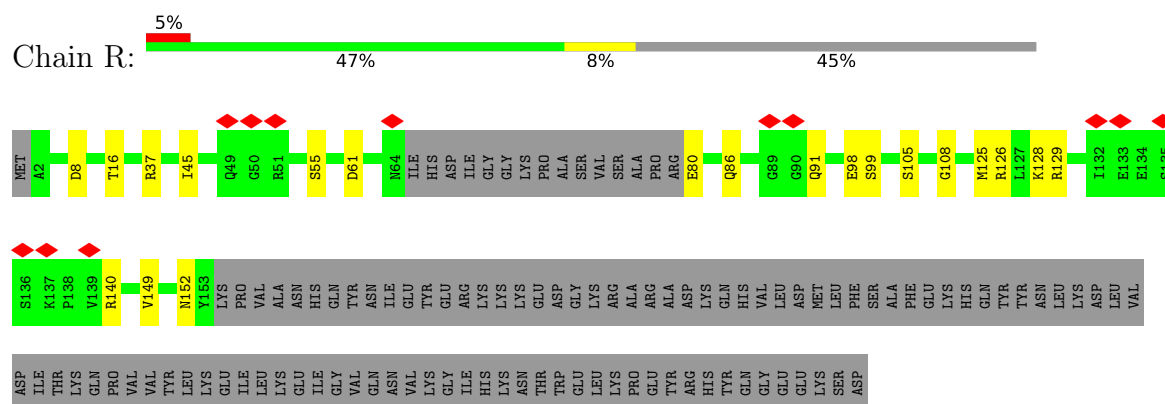


- Molecule 15: General transcription factor IIF subunit 1

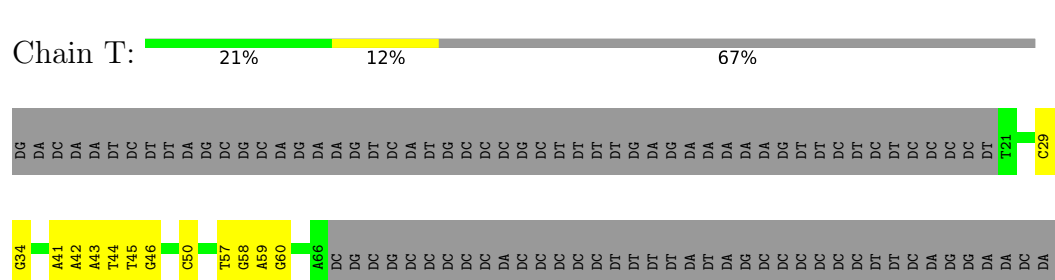
Chain Q:  22% 5% 73%



- Molecule 16: General transcription factor IIF subunit 2

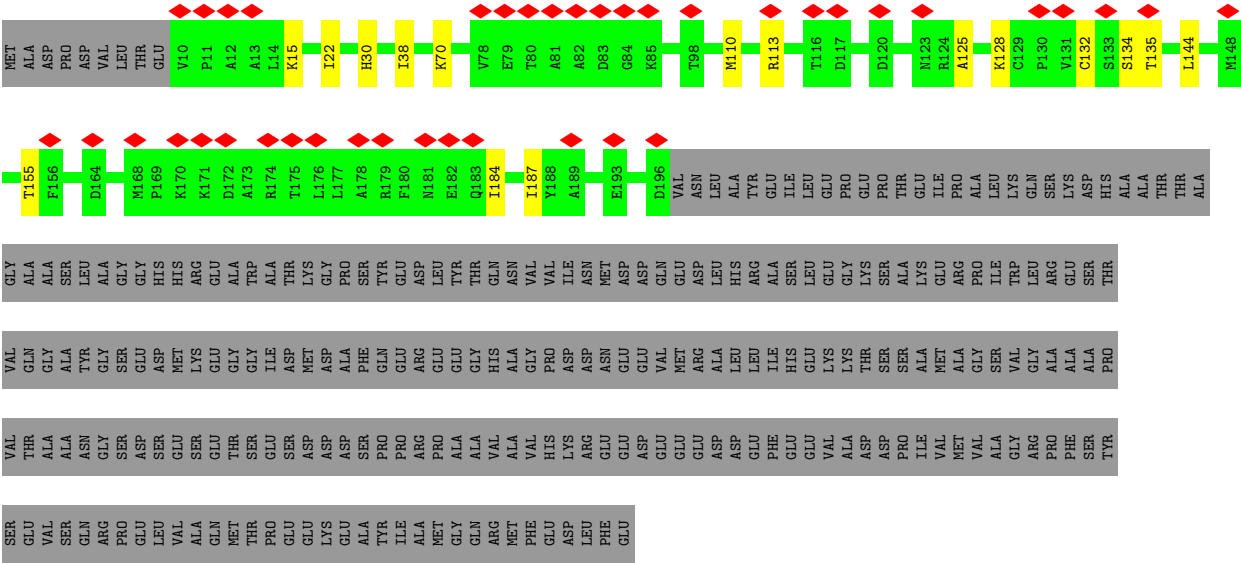


- Molecule 17: Template DNA



- Molecule 18: General transcription factor IIE subunit 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	47.914	Depositor
Minimum map value	-24.547	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.53	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/11439	0.61	1/15440 (0.0%)
2	B	0.22	0/9210	0.57	0/12431
3	C	0.16	0/2102	0.47	0/2857
4	D	0.16	0/1064	0.46	0/1428
5	E	0.24	0/1751	0.62	0/2366
6	F	0.22	0/667	0.64	0/901
7	G	0.16	0/1382	0.47	0/1874
8	H	0.18	0/1207	0.53	0/1628
9	I	0.22	0/948	0.61	0/1284
10	J	0.21	0/542	0.56	0/730
11	K	0.20	0/935	0.51	0/1266
12	L	0.20	0/377	0.62	0/500
13	N	0.66	0/797	0.90	0/1225
14	P	0.66	0/330	0.98	0/511
15	Q	0.18	0/1167	0.51	0/1576
16	R	0.14	0/1083	0.43	0/1459
17	T	0.64	0/1064	0.93	0/1642
18	W	0.18	0/1560	0.50	0/2097
All	All	0.26	0/37625	0.59	1/51215 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	GLN	N-CA-C	5.13	121.73	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	862	ARG	Sidechain
2	B	472	ARG	Sidechain
2	B	812	ARG	Sidechain
2	B	841	ARG	Sidechain

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	11234	0	11365	175	0
2	B	9030	0	9073	146	0
3	C	2059	0	2007	26	0
4	D	1050	0	1033	7	0
5	E	1720	0	1737	32	0
6	F	657	0	684	15	0
7	G	1351	0	1358	12	0
8	H	1186	0	1147	21	0
9	I	927	0	859	15	0
10	J	533	0	553	12	0
11	K	916	0	939	20	0
12	L	372	0	380	3	0
13	N	712	0	395	5	0
14	P	296	0	154	19	0
15	Q	1138	0	1103	18	0
16	R	1070	0	1086	16	0
17	T	949	0	518	14	0
18	W	1535	0	1540	9	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	W	1	0	0	0	0
20	P	1	0	0	0	0
All	All	36745	0	35931	497	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 7.

All (497) 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)
5:E:29:THR:CG2	5:E:32:GLU:CG	2.24	1.15
5:E:29:THR:HG22	5:E:32:GLU:CD	1.74	1.13
5:E:29:THR:CG2	5:E:32:GLU:HG3	1.81	1.11
5:E:29:THR:CG2	5:E:32:GLU:CD	2.28	1.04
3:C:90:CYS:SG	3:C:94:CYS:HB3	1.97	1.03
1:A:557:ARG:O	1:A:561:MET:HB2	1.61	1.00
5:E:29:THR:HG22	5:E:32:GLU:OE1	1.66	0.96
5:E:29:THR:HG21	5:E:32:GLU:HG3	1.48	0.95
1:A:351:ARG:NE	1:A:862:ARG:NH1	2.15	0.95
1:A:351:ARG:CD	1:A:862:ARG:HH11	1.82	0.91
1:A:11:SER:N	2:B:1135:TYR:HH	1.70	0.90
1:A:351:ARG:NE	1:A:862:ARG:HH11	1.77	0.81
5:E:29:THR:HG23	5:E:32:GLU:HG3	1.63	0.81
14:P:12:C:H2'	14:P:13:A:H8	1.47	0.78
5:E:29:THR:HG23	5:E:32:GLU:CG	2.14	0.77
1:A:351:ARG:CD	1:A:862:ARG:NH1	2.49	0.76
1:A:351:ARG:HD2	1:A:862:ARG:HH11	1.49	0.75
5:E:29:THR:HG21	5:E:32:GLU:CG	2.09	0.74
8:H:96:VAL:HG12	8:H:116:VAL:HG22	1.68	0.73
5:E:29:THR:HG21	5:E:32:GLU:CD	2.12	0.70
17:T:41:DA:H2'	17:T:42:DA:C8	2.27	0.70
8:H:90:TYR:HB3	8:H:145:MET:HB2	1.72	0.69
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.74	0.69
3:C:67:ARG:HE	10:J:5:VAL:HG13	1.56	0.69
14:P:10:C:H2'	14:P:11:G:C8	2.28	0.68
2:B:866:ILE:HG23	2:B:867:ILE:HD12	1.76	0.67
1:A:114:CYS:SG	1:A:184:CYS:HB3	2.34	0.67
2:B:796:MET:HG2	2:B:965:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:69:ILE:HG22	9:I:71:ASP:H	1.59	0.67
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.75	0.66
1:A:59:ASP:HB3	1:A:62:GLN:HB2	1.78	0.66
2:B:282:ARG:HD2	9:I:21:ASN:HD21	1.61	0.66
9:I:17:CYS:HB3	9:I:22:ASN:H	1.61	0.66
15:Q:46:ARG:HB2	15:Q:101:ARG:HB2	1.77	0.65
1:A:1401:LEU:HG	1:A:1405:MET:HE2	1.78	0.65
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.79	0.65
1:A:539:GLN:O	2:B:970:HIS:ND1	2.30	0.64
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.62	0.64
14:P:6:C:H2'	14:P:7:A:C8	2.32	0.64
1:A:496:PHE:H	2:B:791:GLU:HB3	1.63	0.64
18:W:144:LEU:HD22	18:W:155:THR:H	1.62	0.64
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.38	0.64
2:B:942:LYS:NZ	14:P:14:A:OP1	2.27	0.63
17:T:30:DC:H2'	17:T:31:DC:C6	2.33	0.63
1:A:359:VAL:HG21	2:B:1106:ARG:HD3	1.80	0.63
2:B:784:SER:HA	2:B:789:ASN:HD21	1.64	0.63
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.81	0.63
5:E:29:THR:HG23	5:E:32:GLU:CB	2.29	0.63
10:J:5:VAL:HG23	10:J:6:ARG:HG2	1.81	0.62
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.32	0.62
1:A:1368:VAL:HG13	1:A:1369:LEU:HG	1.82	0.62
8:H:30:CYS:HB2	8:H:39:LEU:HB3	1.80	0.62
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.82	0.62
1:A:267:GLN:HE21	14:P:4:C:H4'	1.65	0.61
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.82	0.61
5:E:29:THR:CG2	5:E:32:GLU:CB	2.78	0.61
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.33	0.60
2:B:841:ARG:HH11	14:P:3:A:H1'	1.65	0.60
1:A:1180:ASN:HB3	1:A:1183:SER:HB3	1.82	0.60
2:B:146:LYS:O	16:R:152:ASN:ND2	2.34	0.60
1:A:481:THR:OG1	1:A:483:ARG:NH2	2.34	0.60
2:B:1036:LYS:HB2	3:C:194:HIS:HB3	1.83	0.59
1:A:1378:LEU:HD21	1:A:1405:MET:HE3	1.83	0.59
9:I:86:CYS:SG	9:I:87:GLN:N	2.75	0.59
14:P:10:C:H2'	14:P:11:G:H8	1.66	0.59
15:Q:27:ASN:ND2	16:R:98:GLU:OE2	2.35	0.59
8:H:59:VAL:HB	8:H:144:LEU:HB2	1.85	0.59
5:E:151:MET:HE3	5:E:192:LYS:HB2	1.85	0.59
14:P:7:A:H2'	14:P:8:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:LEU:HD22	1:A:1368:VAL:HG11	1.85	0.59
4:D:32:LEU:HA	4:D:84:ARG:HH12	1.67	0.58
1:A:29:ASP:OD2	1:A:33:ARG:NH1	2.36	0.58
5:E:29:THR:HG22	5:E:32:GLU:CG	2.15	0.58
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.36	0.58
2:B:552:ASN:OD1	2:B:553:LEU:N	2.37	0.58
9:I:109:ARG:HH11	9:I:124:THR:HG22	1.69	0.58
15:Q:18:VAL:HG22	15:Q:137:ALA:HB3	1.85	0.58
8:H:39:LEU:HD12	8:H:125:LEU:HD21	1.86	0.58
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.87	0.57
1:A:931:ARG:NH2	1:A:936:GLU:OE1	2.37	0.57
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.52	0.57
1:A:999:ARG:NH1	8:H:103:GLU:OE2	2.38	0.57
1:A:1216:LEU:HB2	1:A:1255:LEU:HB2	1.86	0.57
3:C:220:TYR:OH	8:H:46:GLN:NE2	2.37	0.57
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.69	0.57
2:B:598:VAL:HG12	2:B:600:GLU:H	1.70	0.57
7:G:120:ASP:OD1	7:G:122:ASN:ND2	2.38	0.57
6:F:53:THR:OG1	6:F:116:GLU:OE1	2.23	0.57
13:N:58:DT:H1'	13:N:59:DT:H5''	1.86	0.57
2:B:906:GLN:OE1	2:B:922:ARG:NH1	2.39	0.56
4:D:32:LEU:HD12	4:D:36:GLU:HG2	1.87	0.56
1:A:478:PRO:O	1:A:483:ARG:NH1	2.38	0.56
2:B:283:ASP:O	2:B:287:HIS:ND1	2.30	0.56
2:B:751:LEU:HD21	2:B:776:ILE:HD11	1.86	0.56
1:A:355:MET:SD	2:B:1091:ARG:NE	2.77	0.56
1:A:734:ARG:NH2	9:I:106:ASP:OD1	2.37	0.56
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.88	0.56
2:B:41:ARG:NH1	2:B:45:ASP:OD1	2.39	0.56
2:B:474:THR:OG1	2:B:732:ALA:O	2.22	0.56
6:F:57:MET:HB2	6:F:123:LEU:HB3	1.88	0.56
2:B:31:SER:OG	2:B:766:TYR:OH	2.24	0.56
1:A:529:GLN:NE2	1:A:1097:GLU:OE2	2.39	0.56
2:B:1120:ASN:HB2	2:B:1145:GLN:HB3	1.88	0.55
18:W:132:CYS:HG	18:W:134:SER:HG	1.52	0.55
2:B:1125:MET:HE1	2:B:1156:LYS:HG3	1.87	0.55
2:B:218:THR:HA	2:B:238:SER:HA	1.87	0.55
2:B:611:GLU:OE1	2:B:613:ARG:NH2	2.40	0.55
1:A:544:ALA:HB2	1:A:680:LEU:HD22	1.87	0.55
2:B:551:GLU:OE2	16:R:86:GLN:NE2	2.39	0.55
14:P:8:G:H1	17:T:50:DC:H42	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:HG22	7:G:45:VAL:HG11	1.87	0.55
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.88	0.55
3:C:41:GLU:OE2	3:C:255:LYS:NZ	2.35	0.55
3:C:185:GLU:HB3	3:C:230:TYR:HB2	1.87	0.55
1:A:515:ILE:HG23	1:A:519:ALA:HB3	1.89	0.55
1:A:864:LEU:HD21	1:A:1128:ILE:HD12	1.88	0.55
1:A:923:ASP:OD1	1:A:1052:ARG:NH2	2.36	0.55
1:A:902:GLU:OE2	1:A:985:ARG:NH1	2.34	0.54
1:A:1486:ILE:HB	1:A:1487:PRO:HD3	1.89	0.54
2:B:761:THR:HG23	2:B:763:SER:H	1.71	0.54
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.89	0.54
5:E:133:GLN:HA	5:E:136:LEU:HD13	1.90	0.54
1:A:114:CYS:SG	1:A:184:CYS:CB	2.94	0.54
2:B:273:PHE:HB3	2:B:284:ILE:HD12	1.90	0.54
2:B:274:ARG:HG2	2:B:279:VAL:HA	1.90	0.54
6:F:73:ILE:HG21	6:F:92:ILE:HD11	1.89	0.54
1:A:931:ARG:HA	1:A:939:VAL:HG11	1.90	0.54
14:P:7:A:H2'	14:P:8:G:H8	1.73	0.54
2:B:161:CYS:SG	2:B:162:LEU:N	2.81	0.53
3:C:234:GLU:OE1	10:J:42:ARG:NH1	2.40	0.53
1:A:1189:ASP:OD2	1:A:1258:ARG:NH1	2.42	0.53
1:A:99:PHE:O	1:A:103:THR:N	2.41	0.53
10:J:43:TYR:HA	10:J:46:ARG:HD3	1.91	0.53
11:K:100:LEU:HD21	11:K:104:ARG:HH11	1.73	0.53
1:A:681:LEU:HG	2:B:1030:ASN:HD21	1.73	0.53
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.38	0.53
5:E:171:PRO:HB2	5:E:207:ARG:HD3	1.90	0.53
7:G:92:VAL:HB	7:G:126:PRO:HB2	1.90	0.53
1:A:514:GLU:OE2	2:B:1102:PHE:N	2.42	0.53
1:A:713:VAL:HA	1:A:716:VAL:HG12	1.91	0.53
18:W:125:ALA:O	18:W:128:LYS:NZ	2.42	0.53
3:C:78:ILE:HD11	3:C:127:VAL:HG23	1.91	0.52
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.90	0.52
2:B:929:PRO:O	2:B:948:GLN:NE2	2.42	0.52
2:B:255:ARG:HH12	15:Q:167:ARG:HH12	1.57	0.52
2:B:761:THR:H	2:B:764:MET:HE3	1.75	0.52
2:B:114:ARG:NH1	2:B:184:TYR:OH	2.40	0.52
2:B:625:LEU:HD12	2:B:665:ILE:HB	1.90	0.52
16:R:8:ASP:HB3	16:R:105:SER:HA	1.91	0.52
1:A:499:ASP:OD1	14:P:14:A:H4'	2.10	0.52
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:THR:CG2	5:E:32:GLU:HB2	2.39	0.52
5:E:29:THR:HG23	5:E:32:GLU:HB2	1.91	0.52
1:A:998:PRO:O	1:A:1059:ARG:NH2	2.43	0.52
2:B:550:MET:HB2	2:B:577:HIS:HD2	1.75	0.52
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.91	0.52
17:T:32:DT:H2'	17:T:33:DC:C6	2.44	0.52
15:Q:30:ALA:HB2	15:Q:143:TRP:HE1	1.74	0.51
1:A:659:GLU:OE2	1:A:985:ARG:NH2	2.41	0.51
4:D:44:ARG:HH22	7:G:48:VAL:H	1.58	0.51
13:N:58:DT:H1'	13:N:59:DT:C5'	2.41	0.51
1:A:419:ILE:HB	1:A:427:ILE:HB	1.93	0.51
1:A:979:LEU:HD12	1:A:1041:PHE:HD1	1.75	0.51
1:A:1193:VAL:O	1:A:1197:TYR:HB2	2.10	0.51
2:B:904:VAL:HG12	2:B:923:VAL:HG22	1.92	0.51
8:H:88:PHE:HB2	8:H:144:LEU:HD12	1.91	0.51
1:A:535:MET:O	1:A:669:TYR:OH	2.28	0.51
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.91	0.51
4:D:44:ARG:NH2	7:G:48:VAL:O	2.44	0.51
10:J:31:GLU:OE1	10:J:31:GLU:N	2.44	0.51
17:T:59:DA:H2''	17:T:60:DG:C8	2.45	0.51
1:A:538:VAL:O	1:A:539:GLN:HG2	2.11	0.51
2:B:758:LEU:H	2:B:777:ASN:HD21	1.58	0.51
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.51
11:K:89:ASN:HA	11:K:92:THR:HG22	1.92	0.51
15:Q:31:PHE:HD2	15:Q:37:VAL:HG11	1.75	0.51
18:W:184:ILE:HD12	18:W:187:ILE:HD13	1.92	0.51
1:A:606:HIS:ND1	1:A:639:ILE:O	2.40	0.51
2:B:146:LYS:HD3	16:R:149:VAL:HG21	1.93	0.51
3:C:67:ARG:NH1	3:C:149:LEU:O	2.44	0.51
1:A:749:ARG:HA	1:A:752:THR:HG22	1.93	0.51
2:B:255:ARG:HE	2:B:307:GLU:HG3	1.76	0.51
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.92	0.50
2:B:310:VAL:HG23	2:B:311:ILE:HG12	1.92	0.50
2:B:690:CYS:SG	2:B:691:SER:N	2.84	0.50
2:B:801:VAL:HG13	2:B:929:PRO:HD2	1.93	0.50
1:A:991:GLN:HG2	1:A:996:ILE:HD11	1.93	0.50
1:A:1232:ALA:O	1:A:1236:ASN:ND2	2.44	0.50
17:T:57:DT:H2''	17:T:58:DG:N7	2.26	0.50
1:A:604:ARG:NH2	1:A:643:LYS:O	2.44	0.50
2:B:743:ARG:O	2:B:922:ARG:NH2	2.45	0.50
1:A:1005:HIS:CE1	1:A:1007:ILE:HG12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:PRO:HD2	6:F:58:THR:HG21	1.92	0.50
14:P:5:C:H2'	14:P:6:C:C6	2.47	0.50
1:A:1475:LEU:HA	6:F:104:ILE:HG22	1.93	0.50
2:B:841:ARG:HG2	14:P:2:C:H1'	1.92	0.50
1:A:514:GLU:HA	6:F:63:ALA:HB1	1.93	0.50
11:K:22:ASN:HB2	11:K:32:LEU:HB3	1.94	0.50
1:A:775:LYS:HG2	2:B:974:SER:HB3	1.94	0.49
2:B:808:SER:OG	2:B:1050:ARG:NH2	2.44	0.49
15:Q:12:THR:HB	16:R:45:ILE:HB	1.93	0.49
2:B:395:LEU:HD21	2:B:532:ILE:HG21	1.94	0.49
3:C:116:THR:HG23	3:C:118:ARG:H	1.78	0.49
6:F:119:GLY:N	6:F:122:GLU:OE2	2.44	0.49
1:A:467:MET:HG3	1:A:534:VAL:HG21	1.93	0.49
2:B:324:ARG:HH12	15:Q:164:TRP:HE1	1.60	0.49
9:I:109:ARG:NH1	9:I:125:GLU:O	2.46	0.49
1:A:1201:ASP:OD1	1:A:1201:ASP:N	2.45	0.49
8:H:40:ILE:HG22	8:H:124:ARG:HB3	1.95	0.49
11:K:65:HIS:HE1	11:K:67:LEU:HD23	1.77	0.49
1:A:1218:ARG:HD3	1:A:1255:LEU:HD11	1.95	0.49
5:E:29:THR:HG23	5:E:32:GLU:H	1.76	0.49
7:G:18:PHE:HA	7:G:22:LEU:HD12	1.94	0.49
10:J:1:MET:HA	10:J:55:LEU:HB2	1.94	0.49
3:C:88:CYS:SG	3:C:97:CYS:HB3	2.53	0.49
17:T:31:DC:H2'	17:T:32:DT:C6	2.47	0.49
2:B:217:TYR:H	2:B:239:MET:HB2	1.78	0.49
2:B:285:LEU:HD11	2:B:305:LEU:HD21	1.95	0.49
2:B:566:LYS:HA	2:B:576:ILE:HG22	1.94	0.49
2:B:665:ILE:HG23	2:B:669:GLU:HB2	1.94	0.49
2:B:1091:ARG:HB2	2:B:1103:LEU:HD11	1.94	0.49
2:B:606:ASP:OD2	2:B:613:ARG:NH1	2.46	0.48
7:G:79:PRO:HB3	7:G:104:MET:HE2	1.95	0.48
11:K:77:THR:OG1	11:K:81:TYR:O	2.28	0.48
1:A:844:ARG:NH1	2:B:511:PRO:O	2.46	0.48
1:A:1135:LYS:HG3	1:A:1136:THR:HG23	1.94	0.48
2:B:31:SER:HG	2:B:766:TYR:HH	1.57	0.48
2:B:803:ARG:HA	3:C:70:LEU:HD21	1.95	0.48
1:A:344:LYS:HG3	1:A:345:GLY:H	1.78	0.48
1:A:406:VAL:HG23	1:A:429:LEU:HD11	1.95	0.48
1:A:629:VAL:HG13	1:A:636:ILE:HB	1.95	0.48
2:B:206:TYR:OH	2:B:390:ASN:O	2.24	0.48
2:B:824:ASP:O	2:B:872:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:ILE:HB	1:A:1304:ILE:HD12	1.96	0.48
2:B:474:THR:HG22	2:B:476:ALA:H	1.78	0.48
2:B:404:PHE:O	2:B:408:PHE:HB2	2.14	0.48
1:A:1172:ASN:ND2	1:A:1215:GLU:OE2	2.41	0.48
5:E:74:VAL:HG23	5:E:103:LEU:HB2	1.94	0.48
7:G:112:SER:HB2	7:G:162:SER:HA	1.95	0.48
1:A:538:VAL:HG22	1:A:539:GLN:N	2.28	0.48
1:A:1053:ARG:HH11	1:A:1058:PHE:HZ	1.61	0.48
1:A:1099:ALA:HA	1:A:1102:MET:HE1	1.95	0.48
5:E:77:PRO:O	5:E:107:GLN:NE2	2.47	0.48
8:H:106:THR:OG1	8:H:107:GLU:OE1	2.32	0.48
11:K:46:ILE:HG21	11:K:73:ILE:HD13	1.96	0.48
14:P:12:C:H2'	14:P:13:A:C8	2.36	0.48
6:F:65:VAL:HG13	6:F:104:ILE:HD11	1.95	0.48
11:K:82:SER:HB3	11:K:85:GLU:HG2	1.95	0.48
15:Q:24:LYS:HD3	16:R:99:SER:HB2	1.96	0.48
15:Q:25:LYS:HB2	16:R:98:GLU:HG3	1.96	0.48
2:B:256:ILE:HG21	2:B:369:VAL:HG21	1.96	0.47
8:H:8:ASP:OD1	8:H:9:ILE:N	2.47	0.47
15:Q:166:ARG:HD3	15:Q:170:VAL:HA	1.96	0.47
1:A:606:HIS:HD2	1:A:608:THR:HG22	1.79	0.47
1:A:1049:LEU:HD13	1:A:1054:MET:HE1	1.95	0.47
2:B:735:VAL:HG11	10:J:55:LEU:HD21	1.95	0.47
17:T:59:DA:H2''	17:T:60:DG:H8	1.79	0.47
1:A:849:ASP:OD1	1:A:850:THR:N	2.48	0.47
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.95	0.47
11:K:39:ASP:OD1	11:K:40:HIS:N	2.39	0.47
17:T:45:DT:H2'	17:T:46:DG:C8	2.49	0.47
1:A:629:VAL:HG12	1:A:637:MET:HG2	1.97	0.47
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.96	0.47
2:B:298:MET:HA	2:B:301:VAL:HG12	1.96	0.47
2:B:625:LEU:HD13	2:B:675:LEU:HD11	1.97	0.47
8:H:9:ILE:HA	8:H:57:ARG:HA	1.96	0.47
18:W:22:ILE:HD11	18:W:30:HIS:HB3	1.97	0.47
2:B:239:MET:HE1	2:B:254:GLN:HB3	1.96	0.47
3:C:57:SER:OG	3:C:59:LEU:O	2.32	0.47
8:H:124:ARG:NE	8:H:126:GLN:HE22	2.12	0.47
11:K:16:GLU:OE1	11:K:16:GLU:N	2.47	0.47
11:K:65:HIS:CE1	11:K:67:LEU:HD23	2.50	0.47
17:T:45:DT:H2'	17:T:46:DG:H8	1.79	0.47
1:A:545:VAL:O	1:A:549:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.95	0.47
2:B:765:GLU:HG2	2:B:770:ARG:HE	1.80	0.47
2:B:872:THR:HG22	2:B:889:LYS:HG2	1.97	0.47
1:A:31:LEU:HD11	1:A:254:PRO:HG3	1.96	0.47
1:A:1375:ARG:HD2	1:A:1402:CYS:HB3	1.97	0.47
4:D:135:GLN:OE1	4:D:138:ARG:NH2	2.48	0.47
5:E:9:ARG:HG2	5:E:136:LEU:HD21	1.96	0.47
14:P:6:C:H2'	14:P:7:A:H8	1.77	0.47
10:J:2:ILE:HD13	10:J:56:ILE:HG13	1.97	0.47
17:T:43:DA:H2'	17:T:44:DT:C6	2.50	0.46
3:C:75:SER:HB2	3:C:79:VAL:HB	1.96	0.46
2:B:715:ASP:N	2:B:715:ASP:OD1	2.46	0.46
1:A:1358:THR:HG21	1:A:1380:ARG:HH12	1.80	0.46
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.96	0.46
2:B:403:LEU:O	2:B:407:MET:HG2	2.14	0.46
2:B:851:ASP:HB2	12:L:15:MET:HE3	1.97	0.46
2:B:1111:SER:OG	2:B:1112:ASP:N	2.48	0.46
15:Q:15:VAL:O	15:Q:135:PHE:N	2.48	0.46
1:A:244:ARG:NH1	1:A:246:GLU:OE2	2.48	0.46
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.97	0.46
2:B:113:ALA:HA	2:B:118:LEU:HB3	1.98	0.46
2:B:603:MET:SD	2:B:603:MET:N	2.89	0.46
2:B:591:ARG:HG3	2:B:599:SER:HA	1.97	0.46
6:F:58:THR:OG1	6:F:61:GLU:OE1	2.32	0.46
13:N:58:DT:H2''	13:N:59:DT:H5'	1.96	0.46
16:R:55:SER:OG	16:R:80:GLU:OE2	2.31	0.46
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	1.98	0.46
2:B:699:HIS:HD2	2:B:701:SER:H	1.64	0.46
1:A:550:LYS:NZ	1:A:762:GLU:OE2	2.49	0.46
2:B:217:TYR:HE2	2:B:376:ALA:HA	1.81	0.46
1:A:397:PHE:HB3	6:F:87:THR:HG22	1.98	0.45
1:A:539:GLN:CD	2:B:790:GLN:HB3	2.41	0.45
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.82	0.45
8:H:56:PHE:HA	8:H:148:LEU:HD23	1.98	0.45
1:A:1426:PRO:HA	1:A:1429:LYS:HE2	1.98	0.45
2:B:731:GLN:HB2	2:B:1051:LEU:HD22	1.98	0.45
10:J:46:ARG:O	10:J:50:LEU:HB2	2.16	0.45
2:B:89:GLU:HG2	2:B:127:ASP:HB2	1.97	0.45
13:N:41:DC:H2''	13:N:42:DA:C8	2.52	0.45
8:H:31:GLU:OE1	8:H:31:GLU:N	2.50	0.45
1:A:962:ASP:HB3	1:A:1043:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.99	0.45
2:B:564:ALA:HB3	2:B:576:ILE:HD12	1.99	0.45
1:A:529:GLN:HG2	1:A:1094:SER:HB2	1.99	0.45
1:A:561:MET:CE	11:K:59:ALA:H	2.30	0.45
9:I:35:LEU:HD21	9:I:51:SER:HA	1.97	0.45
1:A:489:THR:HG21	2:B:791:GLU:HG3	1.97	0.45
1:A:1102:MET:HG2	1:A:1120:GLY:HA2	1.99	0.45
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.50	0.45
7:G:87:ALA:HB1	7:G:99:THR:HB	1.99	0.45
15:Q:24:LYS:HG2	15:Q:26:TYR:HE1	1.82	0.45
17:T:33:DC:H2'	17:T:34:DG:C8	2.52	0.45
1:A:186:ARG:HA	1:A:186:ARG:HD2	1.75	0.45
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.34	0.45
3:C:41:GLU:OE2	3:C:171:LYS:NZ	2.50	0.45
9:I:73:SER:HA	9:I:95:VAL:HG11	1.98	0.45
1:A:349:ARG:HH21	1:A:353:ASN:HD22	1.65	0.45
1:A:686:THR:OG1	1:A:687:ILE:N	2.50	0.45
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.99	0.45
1:A:813:ASP:OD2	9:I:98:GLN:N	2.48	0.45
2:B:550:MET:HE1	2:B:574:VAL:HG23	1.98	0.45
6:F:102:ILE:HB	6:F:120:VAL:HG11	1.99	0.45
17:T:44:DT:H2'	17:T:45:DT:C6	2.52	0.45
2:B:288:ILE:HD13	2:B:366:GLY:HA2	1.99	0.44
1:A:883:ILE:HG13	1:A:885:GLN:HG3	2.00	0.44
8:H:91:VAL:HG22	8:H:144:LEU:HD13	1.99	0.44
6:F:69:ARG:O	6:F:73:ILE:HD12	2.18	0.44
14:P:9:C:H2'	14:P:10:C:C6	2.52	0.44
16:R:126:ARG:HH11	16:R:129:ARG:HH22	1.65	0.44
1:A:561:MET:HG2	11:K:51:LEU:HD11	1.99	0.44
1:A:766:PHE:HB3	1:A:781:ILE:HD12	1.99	0.44
1:A:1020:LEU:O	1:A:1034:GLN:NE2	2.51	0.44
1:A:1468:THR:O	6:F:64:ARG:NH2	2.50	0.44
1:A:1454:VAL:HG23	1:A:1464:ALA:HB1	1.99	0.44
2:B:47:PHE:HB2	2:B:155:MET:HE2	1.99	0.44
3:C:146:ASP:OD1	3:C:147:ASP:N	2.51	0.44
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.44
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.83	0.44
15:Q:24:LYS:HG2	15:Q:26:TYR:CE1	2.53	0.44
1:A:756:ALA:HB2	1:A:786:ALA:HB2	1.99	0.44
2:B:195:ILE:HD11	2:B:481:HIS:HE2	1.83	0.44
2:B:450:THR:HG23	2:B:452:ASN:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:VAL:HG21	3:C:127:VAL:HG21	2.00	0.44
1:A:1365:ILE:HA	1:A:1368:VAL:HG12	2.00	0.44
1:A:477:LEU:HD12	1:A:483:ARG:HE	1.83	0.43
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.81	0.43
2:B:526:LEU:HB3	2:B:530:ALA:HB3	2.01	0.43
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.99	0.43
16:R:91:GLN:N	16:R:91:GLN:OE1	2.51	0.43
16:R:125:MET:HA	16:R:128:LYS:HB2	2.00	0.43
1:A:698:THR:O	1:A:702:ILE:HG12	2.18	0.43
1:A:959:MET:HE3	1:A:1047:SER:HA	1.99	0.43
1:A:313:HIS:HA	1:A:316:THR:HG22	2.01	0.43
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.99	0.43
2:B:149:ILE:HG22	2:B:435:ILE:HG21	2.00	0.43
2:B:710:ILE:HA	2:B:764:MET:HE2	2.00	0.43
14:P:7:A:O2'	14:P:8:G:H5'	2.18	0.43
1:A:841:MET:HE1	2:B:503:ASN:HD22	1.84	0.43
1:A:279:LYS:O	1:A:283:ILE:HG12	2.19	0.43
2:B:604:ILE:HD11	2:B:668:LEU:HB3	2.01	0.43
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.43
1:A:538:VAL:HG13	1:A:539:GLN:HG2	2.00	0.43
3:C:86:ARG:HD2	11:K:11:LEU:HD11	1.99	0.43
10:J:30:THR:HG23	10:J:33:ASP:H	1.83	0.43
1:A:421:ARG:NH1	1:A:425:ASP:OD2	2.52	0.43
1:A:1035:GLU:O	1:A:1039:LEU:HB2	2.19	0.43
1:A:706:ILE:HD11	1:A:787:VAL:HG21	2.01	0.43
2:B:26:CYS:O	2:B:30:ILE:HG12	2.19	0.43
2:B:568:PHE:HB2	2:B:613:ARG:HA	2.01	0.43
2:B:570:ASN:HD21	2:B:616:THR:HB	1.84	0.43
2:B:990:SER:OG	2:B:995:GLU:O	2.33	0.43
4:D:58:SER:OG	4:D:59:GLU:OE1	2.36	0.43
1:A:937:ASP:OD1	1:A:937:ASP:N	2.50	0.43
2:B:908:MET:HE2	2:B:920:LYS:HB2	2.01	0.43
1:A:595:ILE:HD11	1:A:675:VAL:HG11	2.01	0.42
2:B:47:PHE:HE2	2:B:154:ILE:HG23	1.84	0.42
5:E:66:ASP:OD1	5:E:67:ASP:N	2.51	0.42
18:W:110:MET:HA	18:W:113:ARG:HB3	2.01	0.42
11:K:78:THR:OG1	11:K:80:ASP:OD1	2.35	0.42
1:A:1361:ASP:OD1	1:A:1362:ILE:N	2.52	0.42
2:B:224:CYS:HB3	2:B:232:THR:HA	2.02	0.42
2:B:271:ILE:HD12	2:B:311:ILE:HG13	2.00	0.42
2:B:455:ASP:OD1	2:B:456:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:70:LYS:HA	18:W:70:LYS:HD3	1.84	0.42
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.49	0.42
1:A:876:ASP:O	1:A:890:ARG:NH2	2.52	0.42
2:B:814:TYR:HD2	2:B:921:ILE:HD11	1.85	0.42
11:K:23:LYS:HE2	11:K:23:LYS:HB2	1.87	0.42
11:K:104:ARG:HA	11:K:107:VAL:HG12	2.01	0.42
18:W:15:LYS:HE2	18:W:38:ILE:HG23	1.99	0.42
1:A:375:ILE:HB	1:A:666:ARG:HG3	2.00	0.42
2:B:986:GLN:HA	2:B:989:VAL:HG12	2.02	0.42
5:E:150:VAL:HG22	5:E:191:VAL:HG12	2.00	0.42
15:Q:100:LEU:HD22	15:Q:110:PHE:HD2	1.84	0.42
1:A:879:VAL:HB	1:A:888:GLN:HB2	2.01	0.42
2:B:90:GLN:HB3	16:R:140:ARG:HD3	2.01	0.42
2:B:827:GLU:HG3	2:B:869:LYS:HE3	2.01	0.42
2:B:903:ILE:HG21	12:L:55:PHE:HZ	1.84	0.42
7:G:116:GLU:HA	7:G:131:MET:HE1	2.02	0.42
14:P:9:C:H2'	14:P:10:C:H6	1.84	0.42
1:A:769:MET:HG2	2:B:970:HIS:NE2	2.34	0.42
16:R:16:THR:HB	16:R:108:GLY:HA3	2.02	0.42
2:B:802:ASP:HB3	3:C:173:HIS:CE1	2.55	0.42
1:A:930:LEU:HD11	1:A:942:VAL:HG11	2.01	0.42
1:A:1224:ARG:HB3	1:A:1226:LEU:HD22	2.01	0.42
3:C:42:VAL:HB	3:C:178:PRO:HG3	2.00	0.42
16:R:126:ARG:HH11	16:R:129:ARG:HH12	1.67	0.42
6:F:51:ARG:HH11	6:F:118:TRP:HA	1.85	0.41
1:A:464:LEU:HB2	1:A:465:HIS:HD2	1.84	0.41
1:A:992:LYS:HA	1:A:992:LYS:HD3	1.92	0.41
1:A:1118:THR:HG23	1:A:1123:ARG:HD3	2.02	0.41
1:A:1123:ARG:HH12	1:A:1360:ASN:HB3	1.84	0.41
2:B:66:ASP:OD1	2:B:66:ASP:N	2.52	0.41
16:R:37:ARG:NH2	16:R:61:ASP:OD2	2.53	0.41
18:W:128:LYS:HE3	18:W:135:THR:HG22	2.02	0.41
1:A:349:ARG:HD3	1:A:353:ASN:HD22	1.85	0.41
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.55	0.41
9:I:91:HIS:O	9:I:93:GLU:N	2.53	0.41
15:Q:19:PRO:HD2	15:Q:138:PHE:HE1	1.85	0.41
1:A:533:PRO:HD3	1:A:654:HIS:CD2	2.55	0.41
1:A:1163:HIS:HE1	1:A:1297:THR:HG22	1.86	0.41
1:A:1347:LEU:HB2	5:E:137:ILE:HG21	2.02	0.41
2:B:761:THR:HG22	2:B:764:MET:HE3	2.00	0.41
1:A:256:PRO:HA	1:A:257:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:LYS:HZ2	2:B:1091:ARG:NH1	2.17	0.41
2:B:381:GLU:OE1	2:B:381:GLU:N	2.53	0.41
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.54	0.41
2:B:607:ILE:HD12	2:B:607:ILE:H	1.85	0.41
2:B:623:ARG:CZ	2:B:625:LEU:HD21	2.51	0.41
1:A:550:LYS:HG2	1:A:639:ILE:HG12	2.01	0.41
1:A:1405:MET:HA	1:A:1412:MET:HB3	2.02	0.41
1:A:1427:LEU:HD23	1:A:1427:LEU:HA	1.84	0.41
2:B:568:PHE:N	2:B:612:ILE:O	2.46	0.41
8:H:103:GLU:N	8:H:103:GLU:OE1	2.54	0.41
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.56	0.41
1:A:1192:TRP:HA	1:A:1195:VAL:HB	2.03	0.41
3:C:68:LEU:HD23	3:C:71:ILE:HD12	2.01	0.41
4:D:33:LEU:HD12	4:D:80:ILE:HG23	2.02	0.41
7:G:41:LYS:O	7:G:78:ARG:NH2	2.54	0.41
9:I:119:CYS:SG	9:I:120:GLY:N	2.77	0.41
1:A:591:ILE:O	1:A:595:ILE:HG12	2.21	0.41
1:A:868:MET:SD	1:A:1404:THR:HG21	2.61	0.41
2:B:282:ARG:HD3	15:Q:34:ALA:HB1	2.02	0.41
5:E:13:ILE:HD11	5:E:132:GLN:HG3	2.01	0.41
1:A:22:GLN:HB3	2:B:1170:ARG:HB2	2.02	0.41
1:A:355:MET:HE2	1:A:355:MET:HB2	1.87	0.41
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.47	0.41
2:B:59:VAL:HG11	2:B:91:ILE:HD11	2.03	0.41
5:E:63:ALA:HB1	5:E:68:PRO:HA	2.03	0.41
5:E:154:GLU:HA	5:E:157:THR:HG22	2.03	0.41
9:I:70:ALA:HB2	9:I:122:ARG:HH11	1.85	0.41
1:A:390:PHE:HB2	1:A:505:LEU:HD21	2.02	0.41
2:B:42:GLN:HE22	2:B:483:ARG:HG2	1.85	0.41
2:B:1118:VAL:HG21	2:B:1171:MET:HB2	2.03	0.41
5:E:91:CYS:HA	5:E:94:MET:HG2	2.03	0.41
5:E:101:ARG:HD2	5:E:126:ILE:HB	2.02	0.41
9:I:116:ALA:HB3	9:I:119:CYS:HB3	2.03	0.41
14:P:1:A:N3	14:P:1:A:H2'	2.35	0.41
17:T:29:DC:H2''	17:T:30:DC:O4'	2.21	0.41
1:A:1040:LEU:HA	1:A:1043:ILE:HG22	2.02	0.40
2:B:1016:SER:HB2	2:B:1022:LEU:HB3	2.03	0.40
1:A:99:PHE:HB3	1:A:248:MET:HE3	2.02	0.40
1:A:560:VAL:HG23	1:A:591:ILE:HD11	2.03	0.40
1:A:682:ILE:HD13	2:B:1030:ASN:HD22	1.85	0.40
2:B:584:MET:HE3	2:B:584:MET:HB3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:GLU:N	2:B:645:GLU:OE1	2.55	0.40
7:G:83:GLU:OE2	7:G:84:VAL:N	2.54	0.40
1:A:351:ARG:CZ	1:A:862:ARG:NH1	2.83	0.40
1:A:400:ASP:OD1	1:A:400:ASP:N	2.53	0.40
1:A:403:GLN:HA	1:A:406:VAL:HG12	2.03	0.40
1:A:988:TRP:HE1	1:A:992:LYS:NZ	2.20	0.40
1:A:1174:ALA:N	1:A:1213:ARG:O	2.51	0.40
1:A:1412:MET:HE2	1:A:1412:MET:HB2	1.84	0.40
2:B:600:GLU:O	2:B:620:ARG:NH1	2.55	0.40
2:B:849:ASP:HB3	12:L:15:MET:HE1	2.03	0.40
10:J:10:CYS:SG	10:J:11:GLY:N	2.94	0.40
13:N:57:DT:H2''	13:N:58:DT:H5'	2.03	0.40
2:B:255:ARG:NH1	15:Q:167:ARG:HH12	2.18	0.40
2:B:407:MET:HE2	2:B:407:MET:HB3	1.90	0.40
2:B:1035:ARG:HA	3:C:28:LEU:HD21	2.04	0.40
5:E:106:VAL:O	5:E:132:GLN:N	2.54	0.40
8:H:87:GLN:OE1	8:H:87:GLN:N	2.40	0.40
2:B:1120:ASN:HD22	2:B:1145:GLN:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1405/1984 (71%)	1322 (94%)	82 (6%)	1 (0%)	48	78
2	B	1122/1300 (86%)	1064 (95%)	58 (5%)	0	100	100
3	C	253/275 (92%)	242 (96%)	11 (4%)	0	100	100
4	D	126/184 (68%)	122 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
8	H	146/150 (97%)	133 (91%)	13 (9%)	0	100	100
9	I	112/125 (90%)	98 (88%)	14 (12%)	0	100	100
10	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
11	K	112/117 (96%)	103 (92%)	9 (8%)	0	100	100
12	L	42/58 (72%)	36 (86%)	6 (14%)	0	100	100
15	Q	134/517 (26%)	127 (95%)	7 (5%)	0	100	100
16	R	133/249 (53%)	131 (98%)	2 (2%)	0	100	100
18	W	185/439 (42%)	184 (100%)	1 (0%)	0	100	100
All	All	4291/5974 (72%)	4061 (95%)	229 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	GLN

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	1249/1763 (71%)	1248 (100%)	1 (0%)	88	89
2	B	990/1127 (88%)	990 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/160 (74%)	118 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
15	Q	121/448 (27%)	121 (100%)	0	100	100
16	R	118/218 (54%)	118 (100%)	0	100	100
18	W	169/373 (45%)	169 (100%)	0	100	100
All	All	3846/5257 (73%)	3845 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	267	GLN
1	A	278	HIS
1	A	353	ASN
1	A	377	GLN
1	A	465	HIS
1	A	493	ASN
1	A	504	HIS
1	A	562	ASN
1	A	576	GLN
1	A	599	HIS
1	A	620	HIS
1	A	671	ASN
1	A	677	ASN
1	A	703	GLN
1	A	740	GLN
1	A	904	GLN
1	A	1032	GLN
1	A	1077	ASN
1	A	1146	GLN
1	A	1163	HIS
1	A	1230	GLN
1	A	1236	ASN

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Mol	Chain	Res	Type
1	A	1360	ASN
1	A	1422	GLN
1	A	1457	ASN
1	A	1462	GLN
2	B	98	HIS
2	B	139	GLN
2	B	164	ASN
2	B	265	GLN
2	B	456	GLN
2	B	460	HIS
2	B	577	HIS
2	B	654	GLN
2	B	683	GLN
2	B	755	GLN
2	B	1021	HIS
2	B	1117	HIS
2	B	1120	ASN
3	C	66	HIS
3	C	190	ASN
3	C	217	GLN
4	D	93	HIS
5	E	116	GLN
5	E	189	GLN
7	G	122	ASN
8	H	46	GLN
8	H	126	GLN
9	I	60	HIS
9	I	91	HIS
11	K	2	ASN
11	K	29	ASN
11	K	40	HIS
15	Q	32	ASN
15	Q	53	ASN
15	Q	103	ASN
15	Q	129	GLN
15	Q	142	ASN
15	Q	173	HIS
15	Q	178	GLN
16	R	64	ASN
16	R	123	ASN
18	W	101	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	13/14 (92%)	3 (23%)	2 (15%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	2	C
14	P	3	A
14	P	7	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	2	C
14	P	6	C

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, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

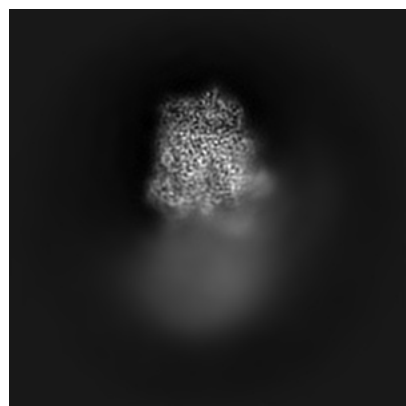
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19720. These allow visual inspection of the internal detail of the map and identification of artifacts.

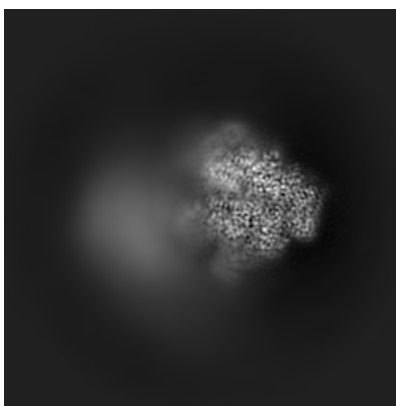
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

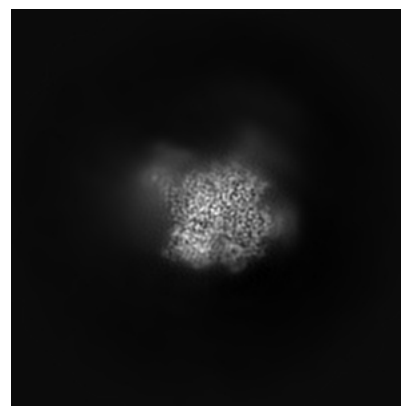
6.1.1 Primary map



X

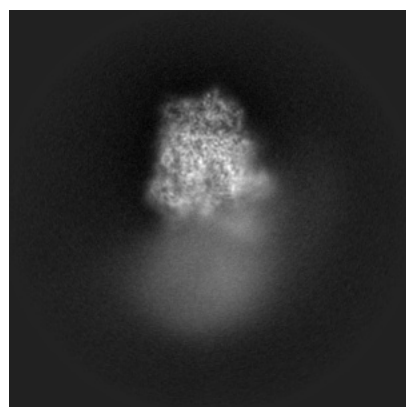


Y

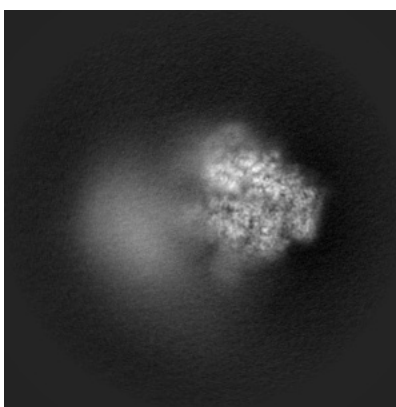


Z

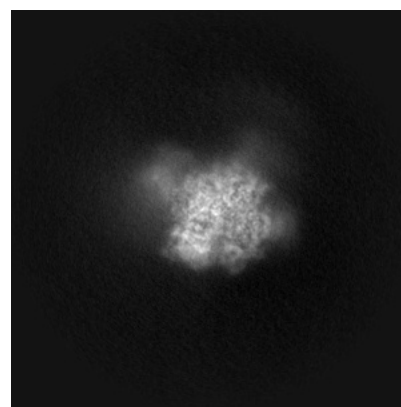
6.1.2 Raw map



X



Y

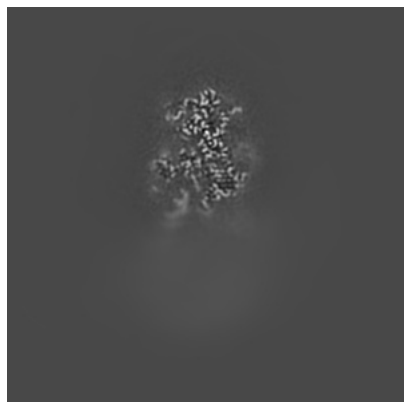


Z

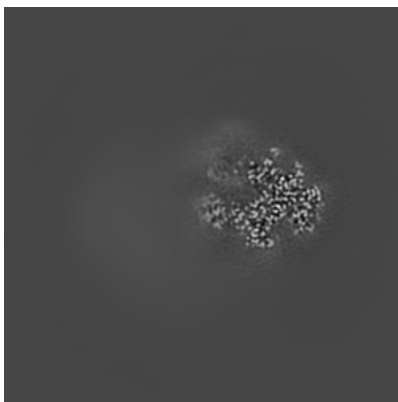
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

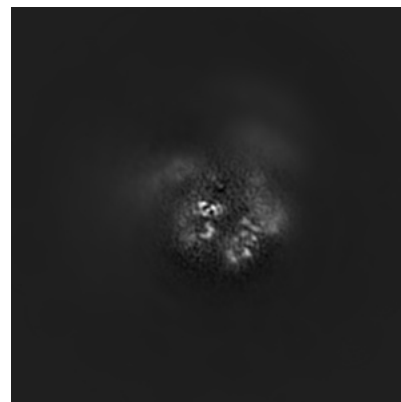
6.2.1 Primary map



X Index: 200

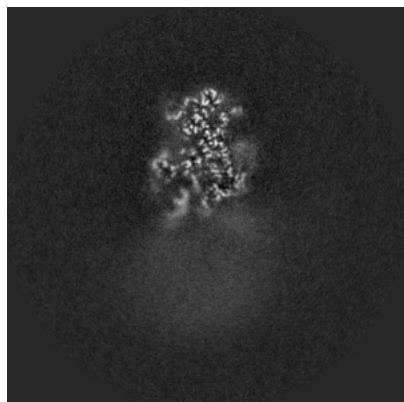


Y Index: 200

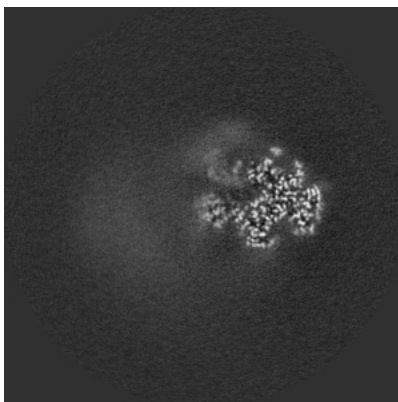


Z Index: 200

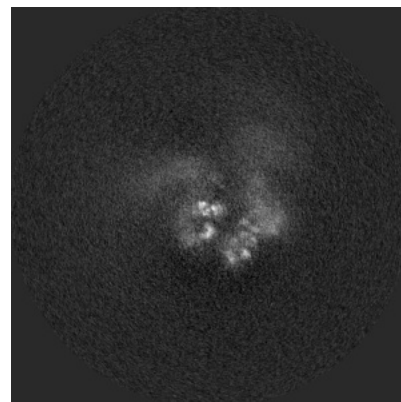
6.2.2 Raw map



X Index: 200



Y Index: 200

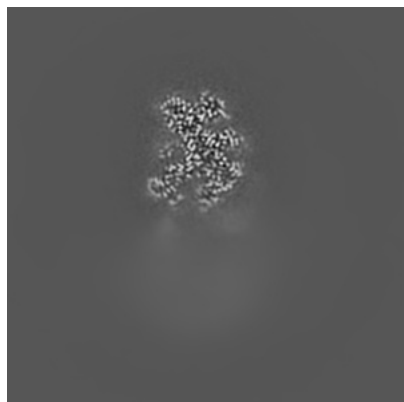


Z Index: 200

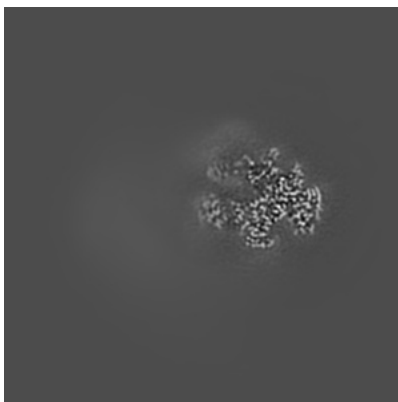
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

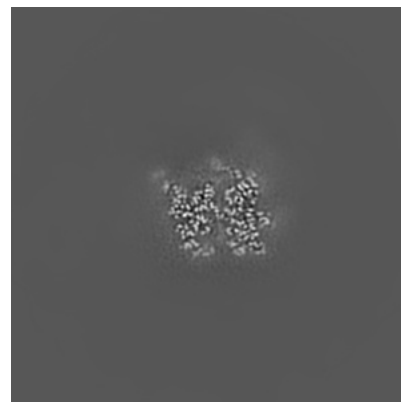
6.3.1 Primary map



X Index: 187

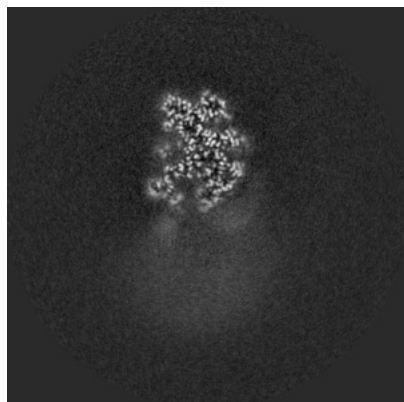


Y Index: 199

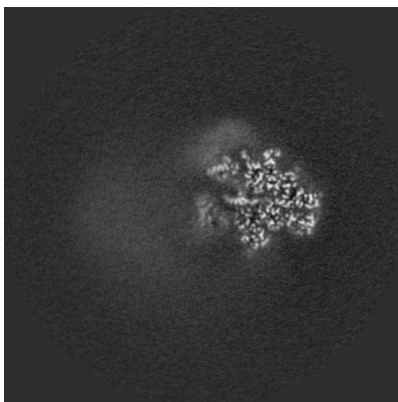


Z Index: 251

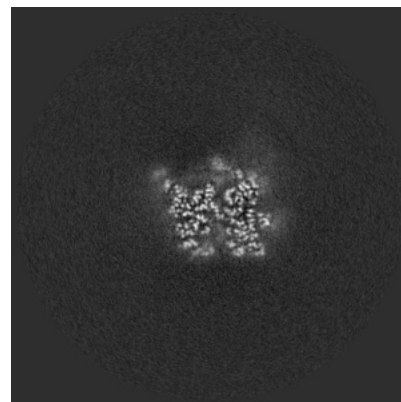
6.3.2 Raw map



X Index: 188



Y Index: 195

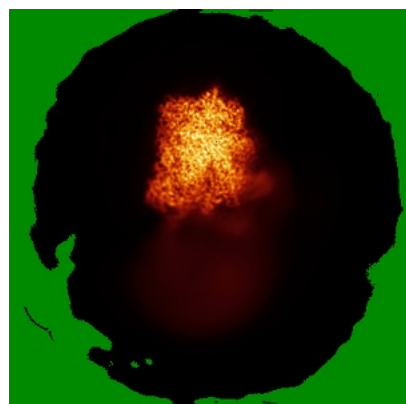


Z Index: 251

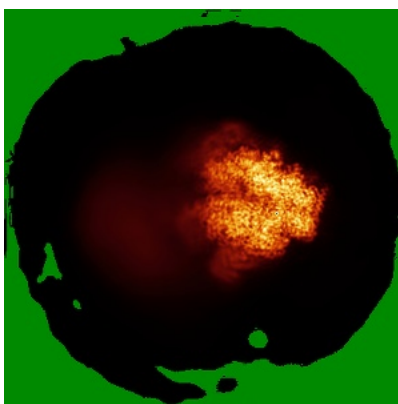
The images above show the largest variance slices of the map in three orthogonal directions.

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

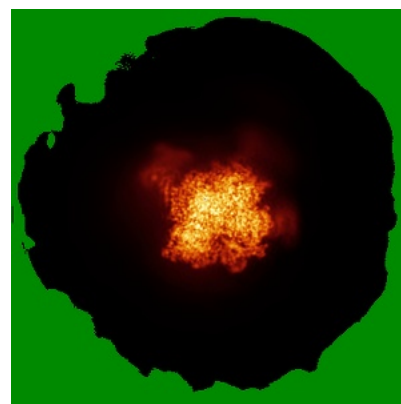
6.4.1 Primary map



X

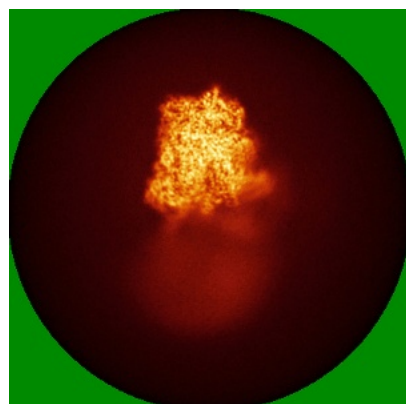


Y

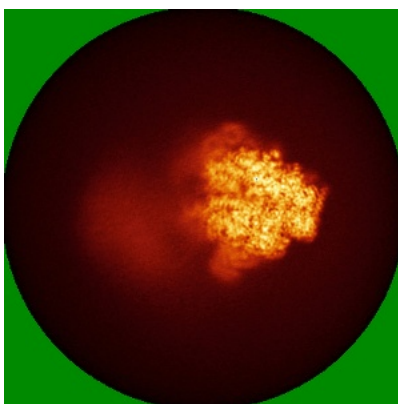


Z

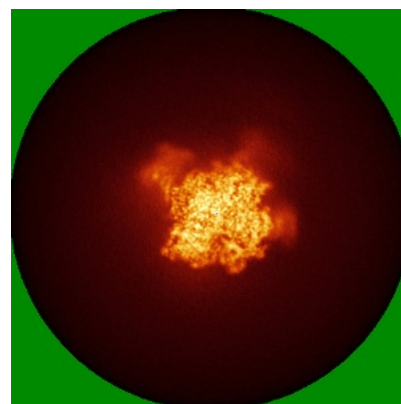
6.4.2 Raw map



X



Y



Z

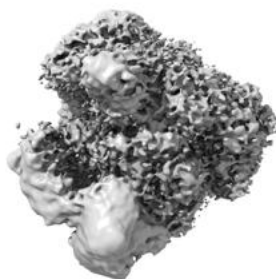
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

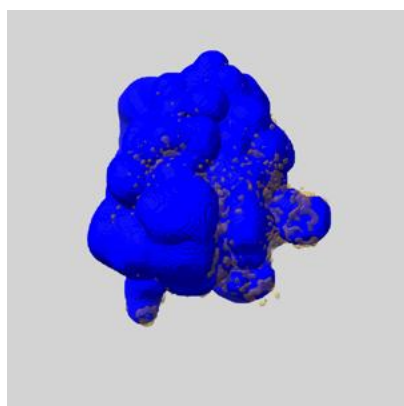
6.6 Mask visualisation [i](#)

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

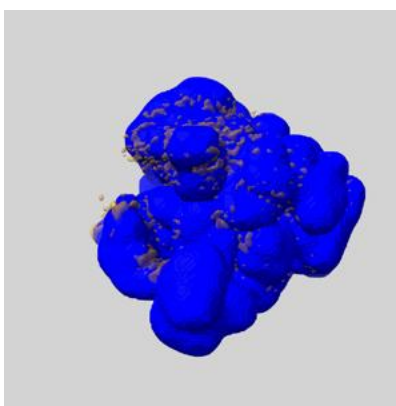
A mask typically either:

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

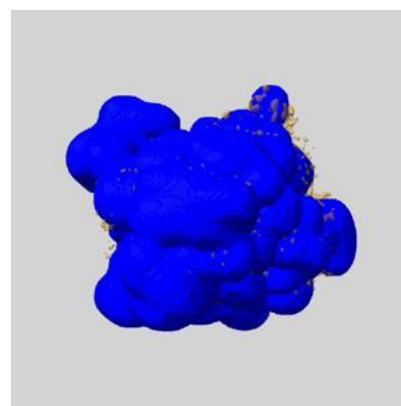
6.6.1 emd_19720_msk_1.map [i](#)



X



Y

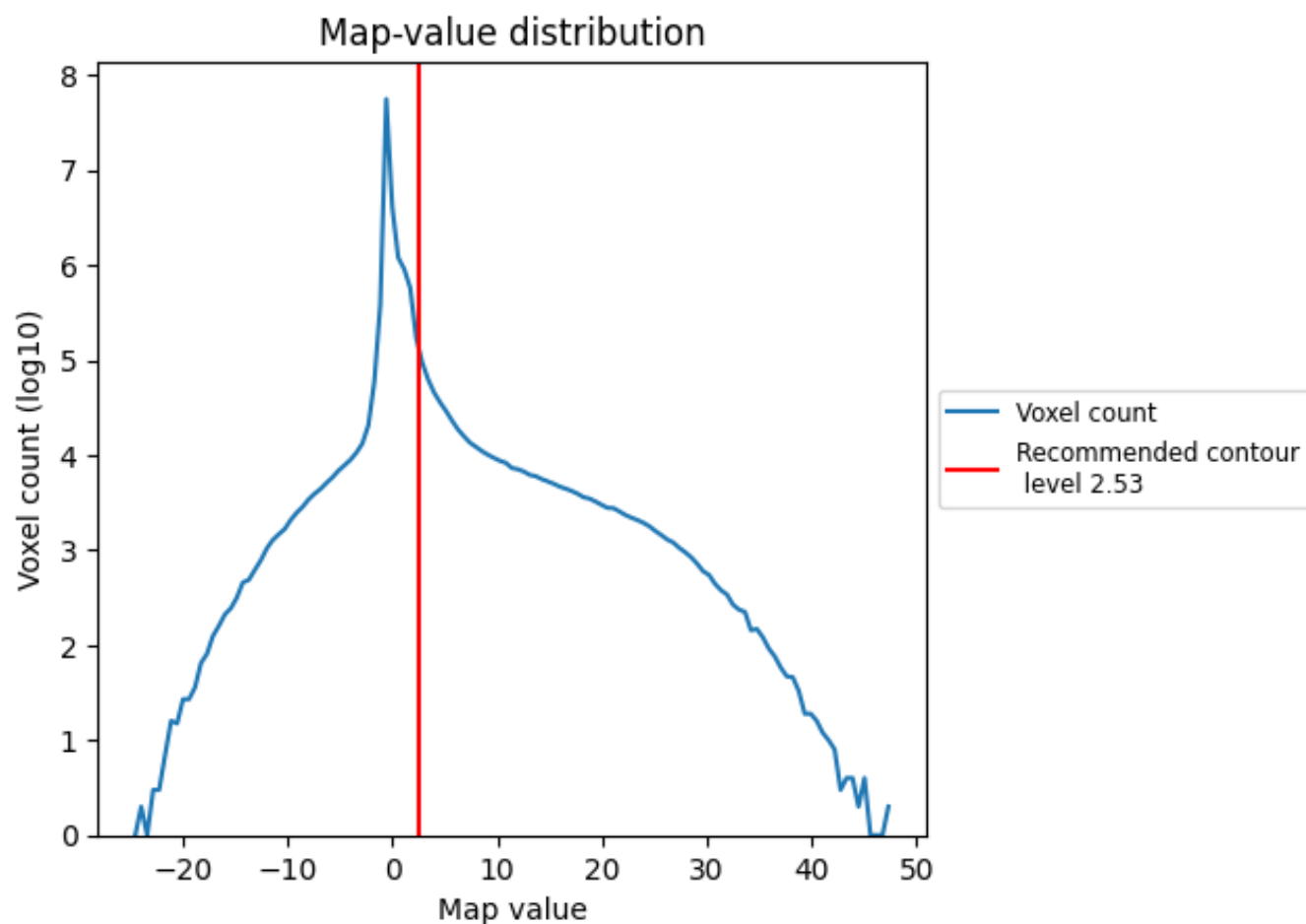


Z

7 Map analysis [i](#)

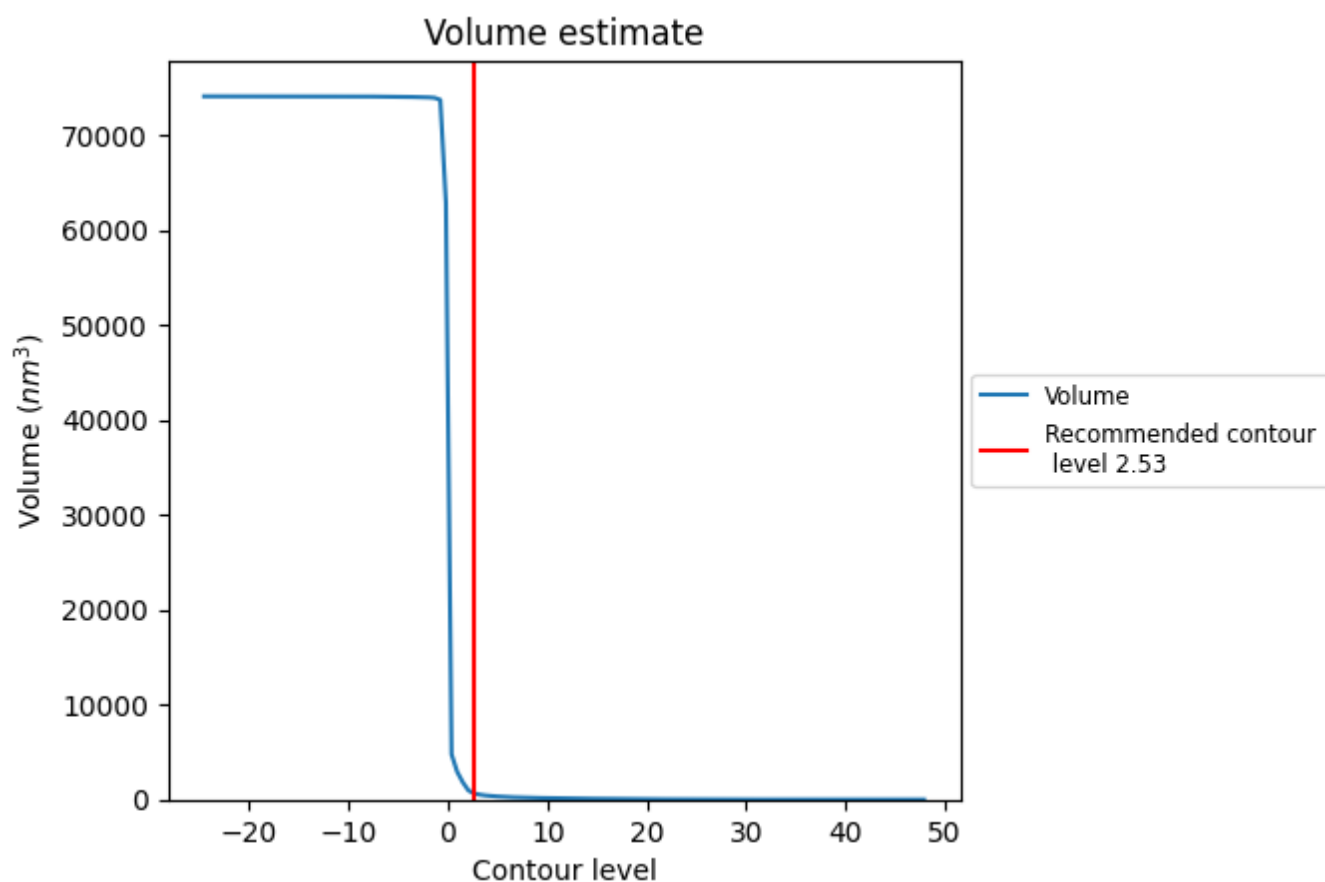
This section contains the results of statistical analysis of the map.

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.

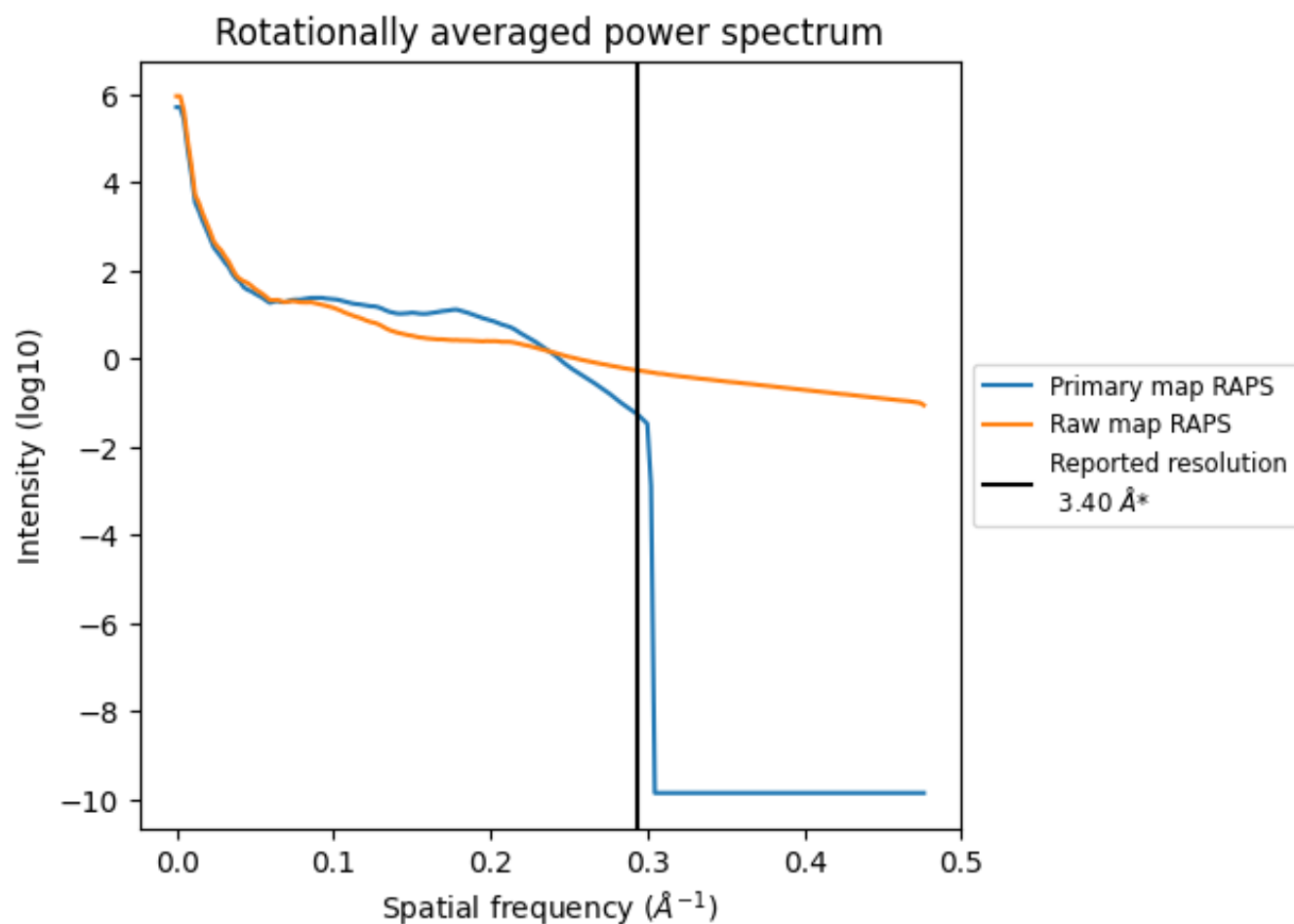
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm^3 ; this corresponds to an approximate mass of 631 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 ⓘ

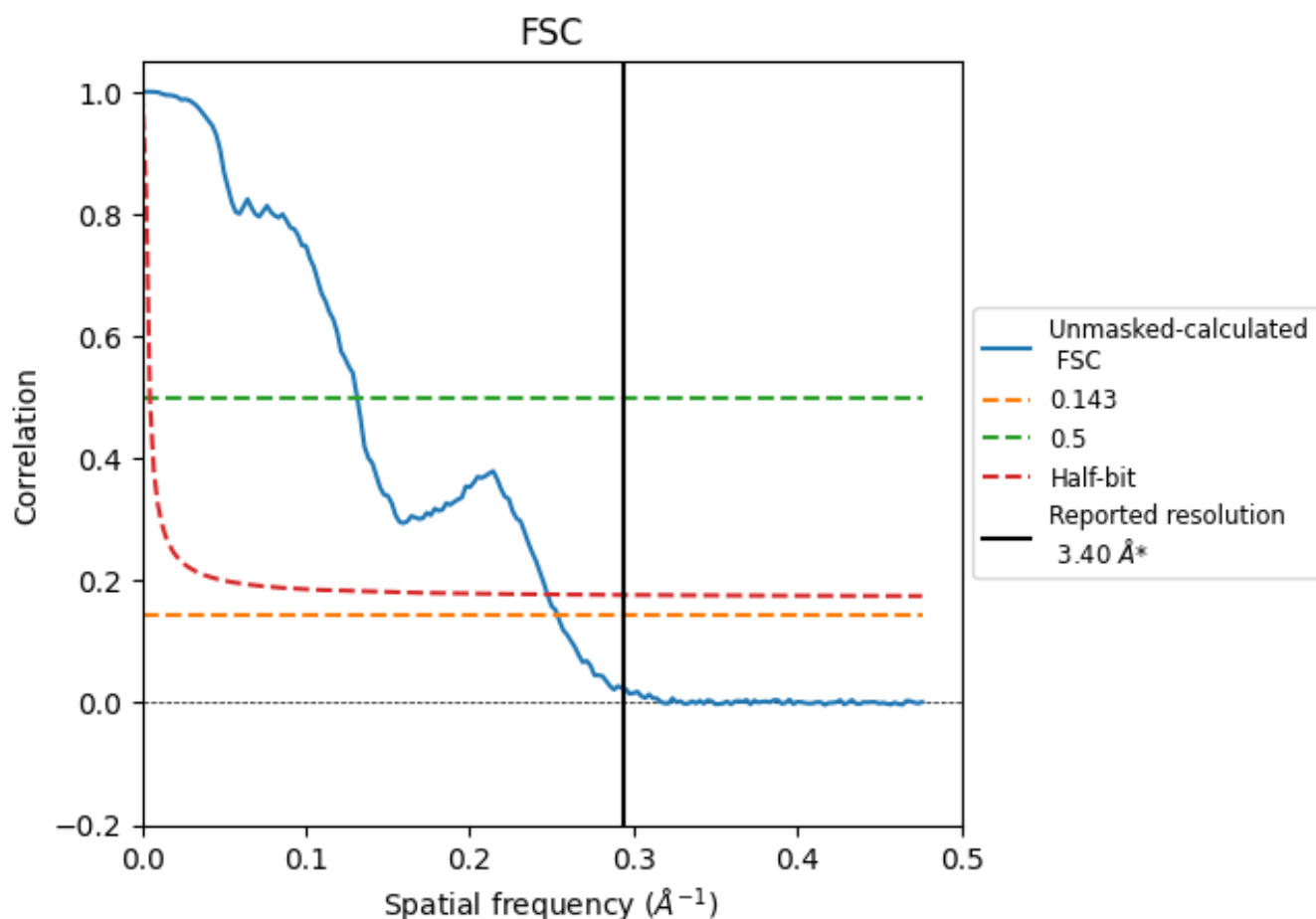


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

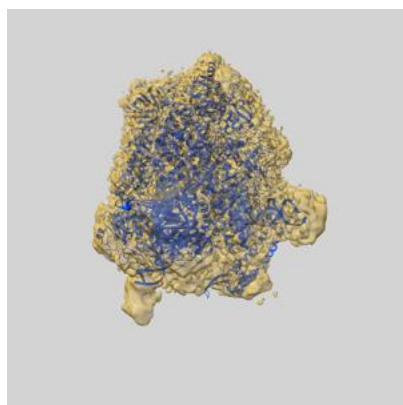
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	7.62	4.04

*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 3.94 differs from the reported value 3.4 by more than 10 %

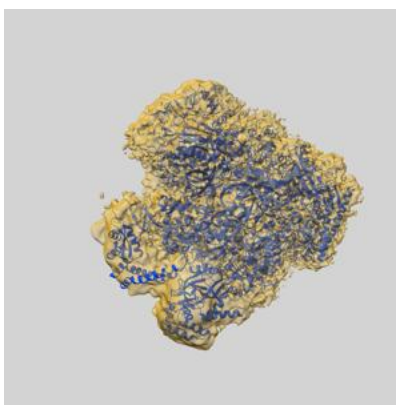
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19720 and PDB model 8S54. Per-residue inclusion information can be found in section [3](#) on page [8](#).

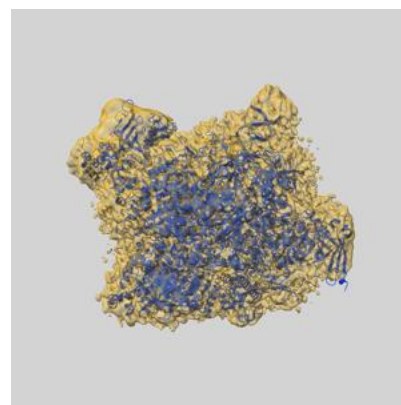
9.1 Map-model overlay [i](#)



X



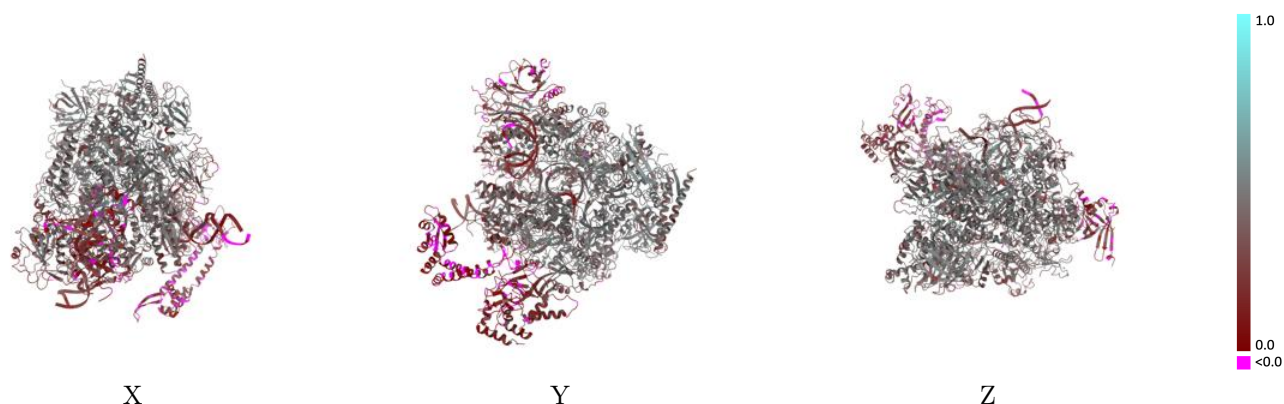
Y



Z

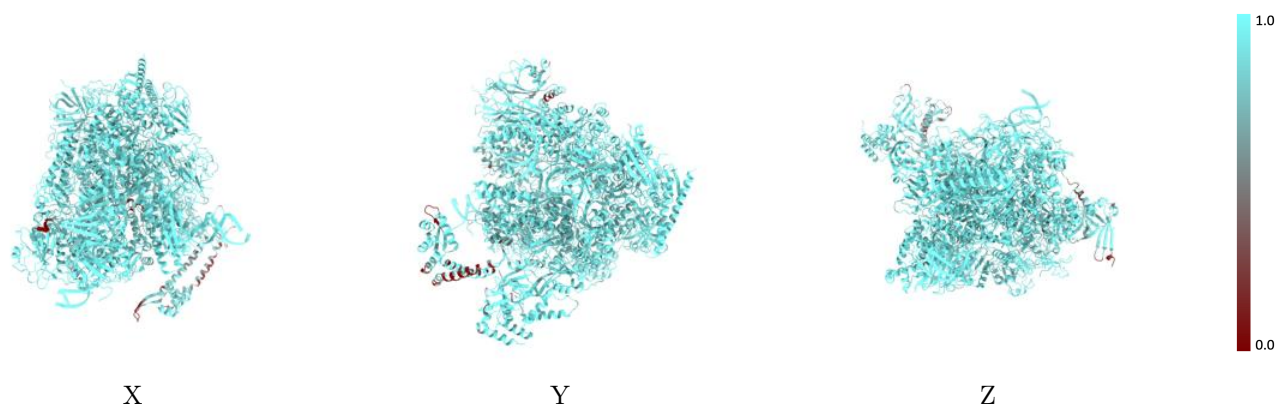
The images above show the 3D surface view of the map at the recommended contour level 2.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



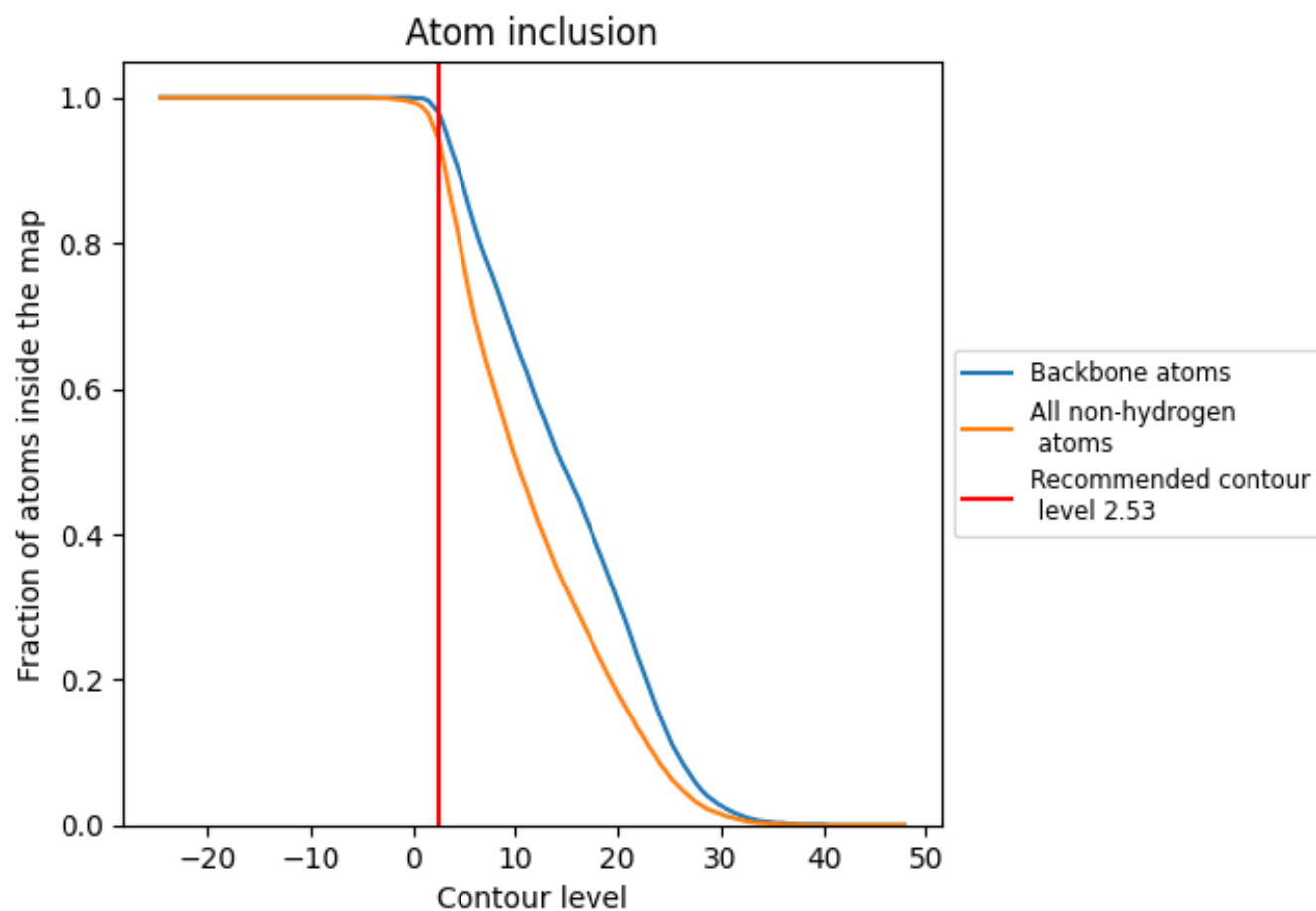
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.53).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (2.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.3680
A	 0.9520	 0.4170
B	 0.9520	 0.4280
C	 0.9710	 0.4540
D	 0.9550	 0.1750
E	 0.9550	 0.3890
F	 0.9610	 0.4170
G	 0.9350	 0.2010
H	 0.9610	 0.4280
I	 0.9590	 0.3760
J	 0.9710	 0.4550
K	 0.9790	 0.4440
L	 0.9330	 0.3130
N	 0.9790	 0.2370
P	 0.9630	 0.3650
Q	 0.8850	 0.1920
R	 0.8560	 0.1490
T	 0.9830	 0.3030
W	 0.7350	 0.0540

