Full wwPDB EM Validation Report (i)

Aug 25, 2026 – 05:32 pm BST

PDB ID	:	8RAP / pdb_00008rap
EMDB ID	:	EMD-19022
Title	:	Structure of Sen1-ADP.BeF3 bound RNA Polymerase II pre-termination complex
Authors	:	Rengachari, S.; Lidscreiber, M.; Cramer, P.
Deposited on	:	2023-12-01
Resolution	:	4.30 Å(reported)
Based on initial models	:	7NKX, ., 2XZO, 6I59

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 (i) 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 (i)) were used in the production of this report:

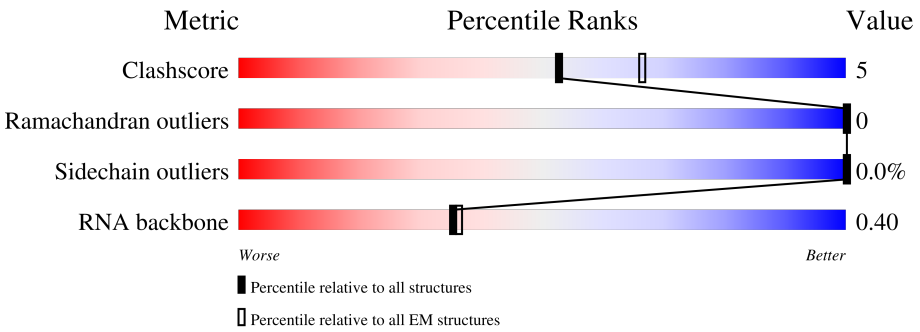
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

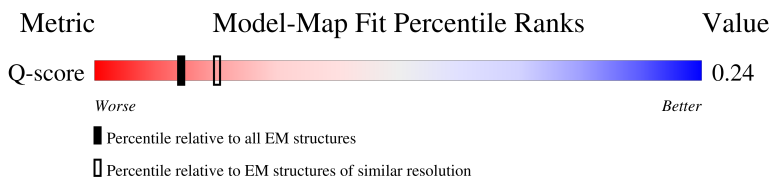
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	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	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	68% 13% 19%
2	B	1224	78% 13% 9%
3	C	318	72% 11% 17%

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Mol	Chain	Length	Quality of chain
4	D	221	63% 9% 28%
5	E	215	86% 14%
6	F	155	48% 6% 45%
7	G	171	88% 12%
8	H	146	82% 10% 9%
9	I	122	87% 10%
10	J	70	83% 10% 7%
11	K	120	78% 18%
12	L	70	56% 6% 39%
13	M	145	40% 5% 55%
14	N	58	41% 5% 53%
15	O	2231	28% 69%
16	P	35	40% 31% 29%
17	T	58	48% 17% 34%
18	Y	102	94%
19	Z	1063	7% 36% 60%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	BEF	O	3003	-	-	X	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 42924 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
			Total	C	N	O	S		
1	A	1400	11020	6948	1929	2081	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1113	8839	5596	1553	1635	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	264	2078	1308	346	411	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	159	1270	788	223	257	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	85	688	439	116	130	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1340	861	222	249	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	133	1068	673	180	211	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	118	964	592	178	184	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	65	532	339	93	94	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	590	157	171	2	0	1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	43	343	211	69	59	4	0	0

- Molecule 13 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	65	504	311	87	101	5	0	0

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	27	547	262	98	160	27	0	0

- Molecule 15 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	694	5557	3509	973	1044	31	0	0

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	P	25	540	240	101	174	25	0	0

- Molecule 17 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	T	38	786	374	142	232	38	0	0

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Y	100	760	474	129	147	10	0	0

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	426	3374	2136	599	630	9	0	0

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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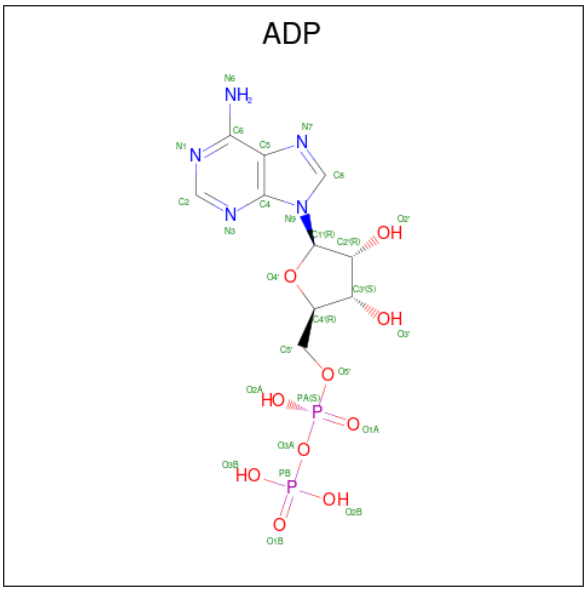
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	C	1	1	1	0
20	I	2	2	2	0
20	J	1	1	1	0
20	L	1	1	1	0
20	M	1	1	1	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

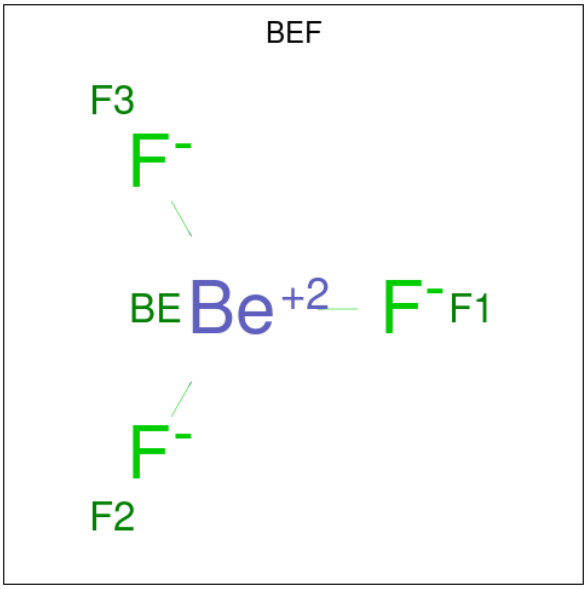
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
21	A	1	1	1	0
21	O	1	1	1	0

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	O	1	27	10	5	10	2	0

- Molecule 23 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



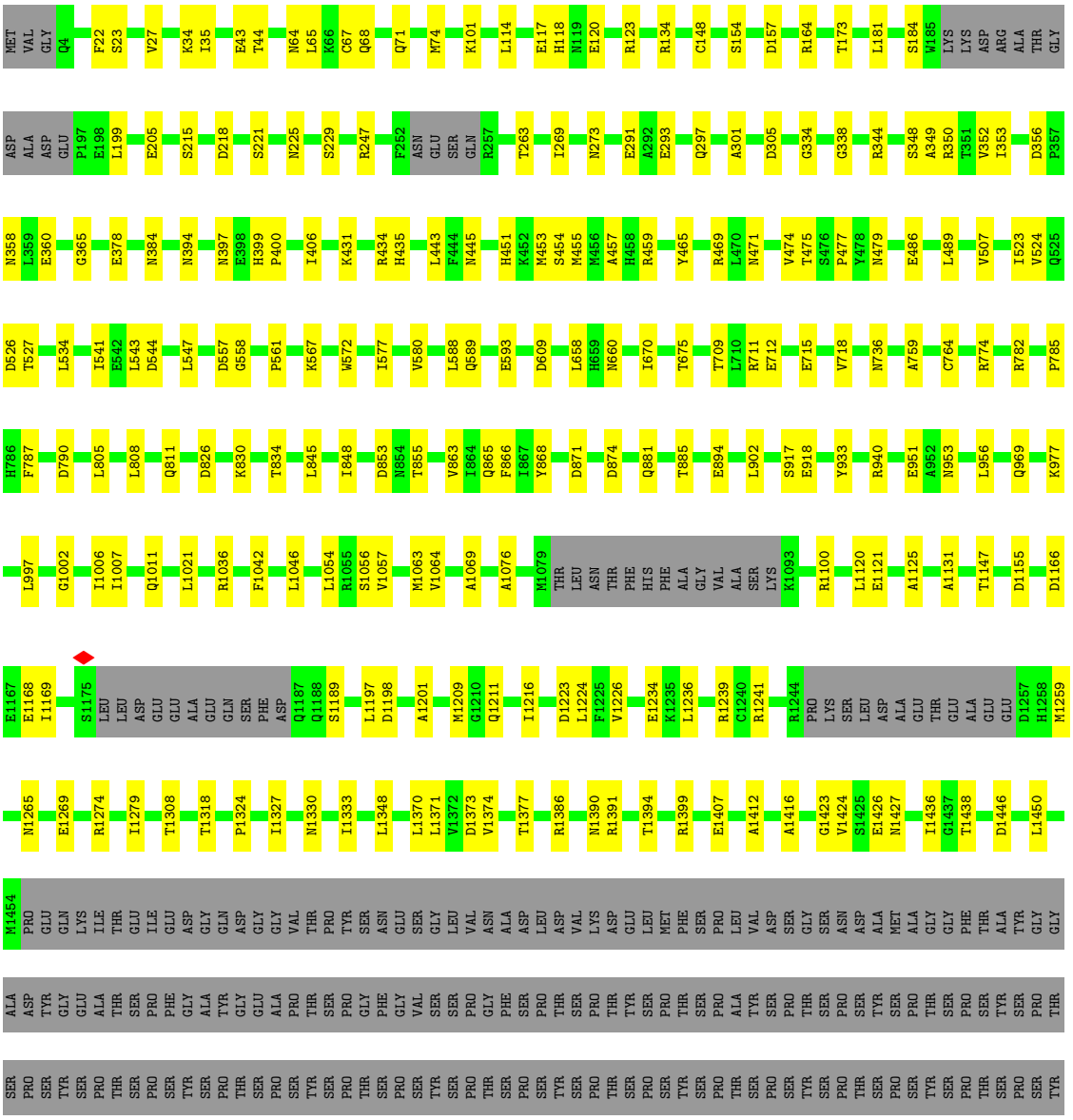
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
23	O	1	4	1	3	0

3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A: 68% 13% 19%



SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER

PRO ASN TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO GLY TYR SER PRO GLY SER PRO ALA TYR SER PRO LYS GLN ASP GLU GLN LYS HIS ASN GLU ASN GLU ASN SER ARG

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

Chain B: 78% 13% 9%

MET SER ASP LEU ALA ASN SER GLU LYS TYR TYR ASP GLU ASP PRO TYR GLY PHE GLU D20 E21 S22 I25 T26 A27 E28 D29 R39 Q53 I70 LEU GLU GLN LEU ALA GLN HIS THR THR GLU SER ASP ASN ILE SER ARG LYS TYR GLU I90 T98 M101 R120

N121 L122 S125 S126 K134 ARG THR TYR GLU ALA ILE ASP VAL PRO GLY ARG GLU LEU LYS TYR GLU LEU ILE ALA GLU GLU SER GLU ASP ASP SER GLU SER GLY K164 R169 E183 K228 I234 Q255 V256 K257 L258 Y259 G260 R261 E262 R267 T268 I269 D279

R287 I292 I301 M310 L314 K315 E319 F322 V323 I324 Q325 D326 R327 E328 L331 R337 L341 Q357 I364 T365 E368 G379 I382 L386 D399 F417 K418 E437 GLU ALA HIS ASP PHE ASN MET LYS L446 E468 Q481

Y488 L492 R496 N499 T500 K510 S540 V547 E564 P565 L566 E567 V570 F581 W586 R604 N610 V613 D618 I619 K622 I626 I639 V640 K649 E650 L651 R654 I658 E665 D668 ILE GLU GLY GLY PHE GLU

ASP VAL GLU E678 G688 E691 M705 E711 P712 ALA GLU ALA ASN GLU GLU ASN ASP LEU ASP VAL D724 R728 H733 T737 D760 H761 N762 Q763 R766 M773 Q776 Y785 N786 T805 T806 R807 E816 N822 A823 I824 A828 Y833 N834

Q835 S845 L850 F851 R857 S858 D861 Q862 M868 S869 E872 R904 V905 S906 G907 E908 S919 PRO ASP GLU GLU GLU LEU GLY GLN ARG THR ALA TYR HIS S933 V952 T956 N957 V966 R967 T971 I976 R983 H984 G985 Q986 K987 R995 R996

N1013 P1014 H1015 E1028 A1035 A1036 L1037 S1038 G1039 N1040 E1041 S1045 Q1065 S1066 R1067 M1082 A1083 Q1084 I1085 R1094 I1103 H1104 R1116 E1120 G1121 R1122 G1126 G1127 L1128 R1129 I1139 L1168 K1174 L1175 N1176 H1177 N1178 M1208 S1221 ARG ASP PHE

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

Chain C: 72% 11% 17%

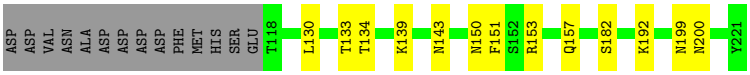
MET SER GLU E4 R11 E12 N17 L33 R34 R35 V36 M37 I38 D47 T53 L58 E61 M75 D90 L101 Q102 E108 T111 V121 K154 L155 I176 E215 D226 T227 N231 S234 I238 V244 V245 R246 G247 I248

I258 L259 L260 Q267 ASP LYS VAL ASN PHE ALA SER GLY ASP ASN ASN THR ALA SER ASN MET LEU GLY SER ASN GLU ASP VAL MET MET THR GLY ALA GLU GLN ASP PRO TYR SER ASN ALA SER GLN MET GLY ASN THR GLY SER GLY GLY TYR ASP ASN ALA TRP

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

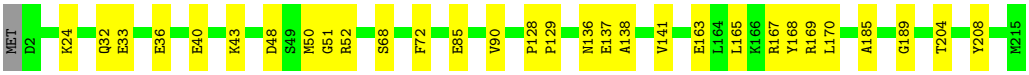
Chain D: 63% 9% 28%

MET ASN VAL SER THR SER THR PHE GLN THR ARG ARG ARG ARG LEU LYS LYS VAL GLU GLU GLU E22 L27 Q28 Q34 Q41 E45 K76 HIS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR THR ALA VAL GLU ASP GLU ASP ASP ASP LEU ASP GLU



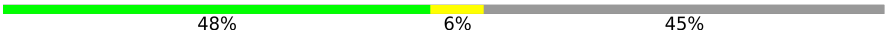
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

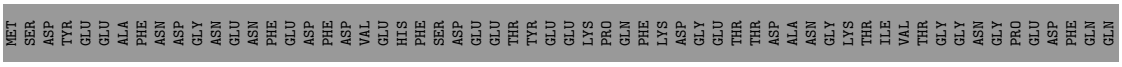
Chain E:

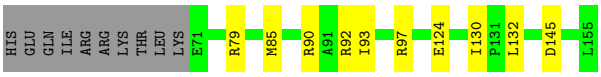


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

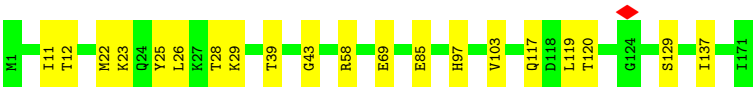






• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

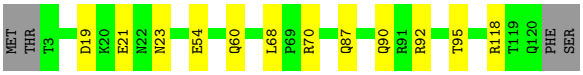


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

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

Chain I:

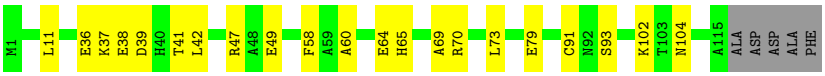


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

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

Chain K:

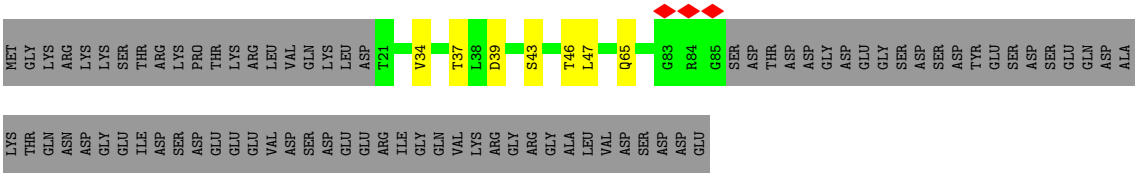


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

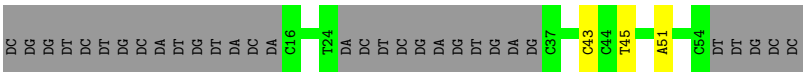
• Molecule 13: Transcription elongation factor 1

Chain M:



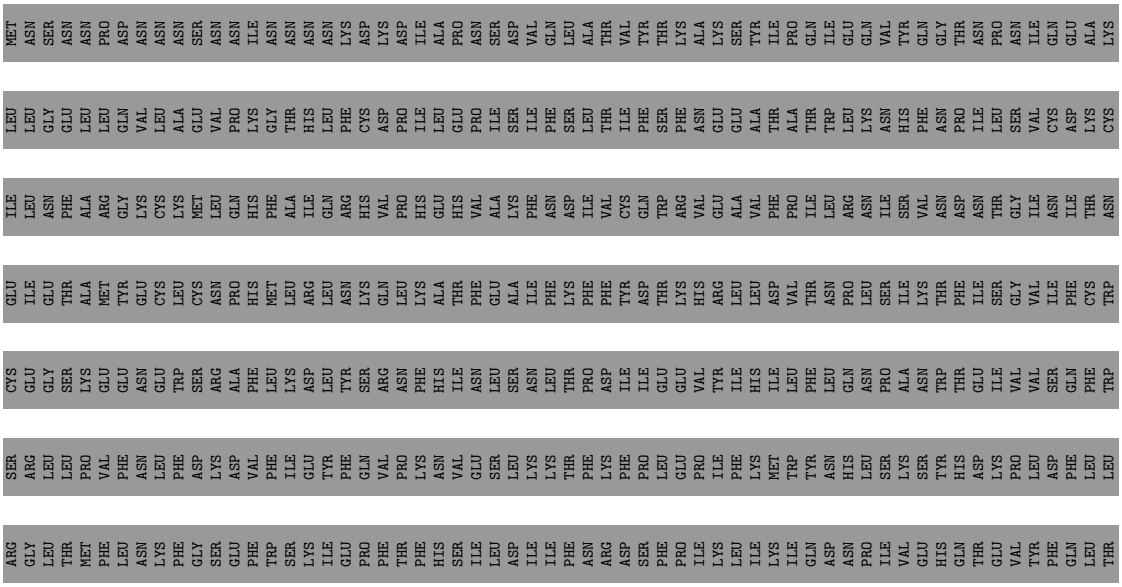
• Molecule 14: Non-template strand

Chain N:



• Molecule 15: Helicase SEN1

Chain O:



ASP	VAL	LYS		S1570	ILE		THR	ALA	ALA	GLN	ASN	ASP	GLN	ALA	PRO	ALA	ALA	GLY
ASP	VAL	LYS	L1843		ARG	Q1309	VAL	ARG	SER	ALA	MET	THR	ARG	ASP	LEU	SER	VAL	SER
ASP	GLY	GLU		H1574	THR		ASP	MET	SER	SER	LEU	ILE	LEU	GLU	LEU	VAL	LEU	VAL
ASP	LYS	LYS	A1854	D1575	ASP	A1313	ILE	GLN	SER	GLU	TYR	TYR	ILE	ASP	ALA	ALA	THR	THR
GLU	LYS	LYS		V1576	PRO	K1314	ASN	LEU	ALA	ILE	TRP	LYS	ASN	ALA	LYS	THR	ILE	ASP
ASP	LYS	LYS	N1876		GLU	P1315	GLY	LEU	GLU	LEU	LEU	PHE	CYS	SER	GLN	SER	LYS	LEU
ASP	ASN	SER	VAL	E1591	LEU		LYS	ASN	SER	GLN	ARG	THR	GLU	GLN	LEU	THR	GLU	LEU
TYR	ASN	LYS	PRO		GLU	S1332	VAL	ASN	ARG	LYS	LEU	LEU	PHE	GLY	LEU	MET	ASN	SER
THR	LYS	ALA	VAL	Q1619	ARG		VAL	ARG	ALA	ALA	SER	LYS	TYR	PHE	VAL	MET	GLU	TRP
PRO	HIS	ASP	PRO		LYS	Q1339	LYS	VAL	ASP	LYS	ASP	TRP	GLU	TRP	SER	VAL	ARG	THR
SER	VAL	ASP	SER	R1641	PHE		ARG	VAL	TYR	ILE	GLU	ALA	PRO	SER	LEU	LEU	ALA	LEU
ILE	CYS	LYS	GLU	M1642	ASN	L1354	GLN	HIS	LEU	PHE	VAL	SER	CYS	CYS	LYS	ALA	MET	PRO
SER	PHE	LYS	GLN		ASN		THR	PRO	GLN	ASN	LEU	LYS	PRO	ILE	ASN	GLU	LEU	PHE
ASP	SER	LYS	GLU	N1645	ALA	T1361	ALA	PRO	ARG	LYS	LEU	TYR	ARG	PHE	ILE	CYS	TYR	TYR
SER	ASP	ASN	ASP		VAL	G1362	A1095	SER	LYS	ALA	GLU	ASP	ALA	SER	ASN	ILE	LYS	HIS
SER	ASP	ASN	ASP	Q1654	THR			ALA	ALA	LEU	SER	TYR	VAL	SER	GLY	ASP	ASN	ALA
LEU	VAL	LYS	TYR		LYS	T1366	Y1125	PRO	LEU	THR	CYS	SER	ARG	ASP	LEU	PHE	ASP	LEU
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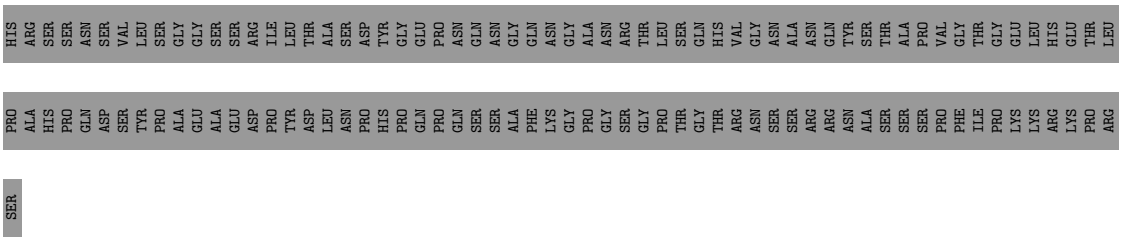
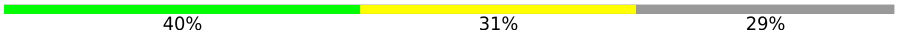
LYS	PHE	ALA	LEU		ARG	T1377	R1127	PHE	SER	GLU	ARG	LEU	LEU	HIS	ILE	ILE	PHE	PRO
SER	ILE	GLU	PRO	Q1671	GLU	LYS	N1128	HIS	SER	VAL	LEU	GLU	MET	LEU	VAL	LEU	GLU	SER
GLU	PRO	SER	MET		LEU	ASN	S1129	THR	ILE	ALA	ILE	ASN	ASP	TYR	PRO	LEU	THR	LYS
ALA	ARG	PRO	GLU	D1676	ARG	ALA		LYS	THR	THR	ILE	PHE	VAL	GLN	SER	LEU	VAL	ARG
ASN	ASN	SER	TYR		GLY	SER	D1134	SER	GLY	GLU	SER	THR	VAL	ALA	ASN	CYS	LEU	ILE
GLY	ASP	THR	ILE	R1686	LYS	SER		ARG	ARG	ALA	THR	LYS	SER	ALA	THR	HIS	LEU	GLN
ARG	GLU	SER	THR		LEU	SER	I1137	GLY	PRO	GLU	SER	ASP	ALA	THR	ALA	ARG	THR	MET
ASN	PRO	SER	GLN	F1699	ASP	ASN		LEU	ARG	ASN	ASP	THR	PHE	ASN	VAL	THR	LYS	VAL
ASN	GLU	GLY	GLY		SER	VAL	Q1167	SER	VAL	TYR	LEU	LEU	VAL	ILE	ALA	PHE	THR	ARG
ARG	ILE	THR	PRO	I1702	GLU	ILE	G1168	ASN	ALA	ARG	ALA	ASP	ASP	LEU	GLU	LYS	ASP	LYS
VAL	LYS	LYS	ASP		SER	LYS	L1169	LYS	GLN	LYS	HIS	LEU	PRO	TYR	ALA	LEU	SER	VAL
ALA	VAL	LYS	GLU	Q1707	GLY	VAL		ASN	PRO	GLU	GLU	SER	ILE	ASN	HIS	TYR	ARG	SER
SER	THR	LYS	VAL		ASN	PRO	R1173	ASP	LYS	LYS	LYS	ARG	SER	THR	ASN	SER	ALA	MET
HIS	ARG	SER	LYS	Y1731	PRO	LEU		ASP	ILE	GLU	HIS	SER	GLY	PHE	ALA	GLY	LEU	ALA
ASN	SER	SER	SER	L1732	GLU	GLU	I1183	SER	THR	LEU	VAL	LEU	VAL	ASP	LEU	LYS	LEU	PHE
GLN	LEU	ILE	ASN	F1733	SER	LYS		SER	SER	SER	LYS	VAL	PHE	VAL	ASN	PRO	ASN	LEU
ASN	SER	PHE	LYS	R1734	PRO	ASN	N1187	SER	PHE	ARG	VAL	ASP	ALA	GLU	GLN	ILE	ASN	ARG
PHE	SER	GLY	ASP	K1735	MET	SER	R1188	GLU	GLY	LEU	ASP	SER	ASN	GLY	LYS	SER	PRO	ILE
SER	VAL	GLY	THR	F1736	SER	SER		GLU	THR	GLY	ASP	PHE	PHE	ARG	PHE	GLU	LEU	ILE
ALA	LEU	MET	LYS	D1737	THR	ASN	V1191	SER	PHE	LYS	SER	ARG	GLN	LEU	LEU	ILE	ILE	ALA
SER	LYS	SER	LYS		GLU	THR		ASP	GLN	VAL	LEU	GLU	THR	GLU	LEU	PRO	GLN	ASN
ILE	GLU	VAL	ARG	I1749	ASP	GLU	F1194	ASN	SER	ILE	VAL	PHE	LEU	GLY	LEU	ILE	ASP	TYR
TYR	LYS	PRO	ARG		ILE	GLN		ASP	SER	ASP	GLU	SER	LYS	ILE	SER	SER	ILE	PRO
ASP	GLN	SER	VAL	M1770	SER	LEU	V1201	ILE	ALA	LEU	MET	ASP	SER	LEU	THR	THR	ILE	SER
ASP	LEU	ALA	VAL		LYS	LEU		GLU	ASN	THR	MET	ILE	GLN	ALA	ARG	ASN	ILE	LEU
PRO	GLY	VAL	ASP	D1776	LEU	LYS	S1212	SER	ALA	ASP	ALA	LEU	ASN	ILE	LEU	VAL	ARG	LYS
GLN	LEU	VAL	GLU	F1777	GLN	K1403		ALA	LYS	SER	LYS	HIS	THR	LEU	MET	LEU	SER	SER
VAL	LYS	PRO	GLY	N1778	LEU		D1215	ARG	LEU	VAL	TYR	ASP	GLU	ASN	GLU	GLU	ALA	ILE
SER	GLU	LYS	GLU	T1779	LYS	I1408	L1216	GLU	HIS	PRO	ALA	GLN	LYS	SER	LYS	ASN	SER	PRO
GLN	THR	THR	GLU		ILE			LEU	ARG	ALA	SER	THR	GLU	ASN	PHE	VAL	ASN	LYS
ALA	ARG	PHE	ALA	F1783	ARG	K1430	A1245	PHE	THR	SER	LYS	LYS	PHE	LEU	ALA	THR	PRO	ALA
LYS	THR	PRO	ASP		GLU	Q1431	K1246	ALA	LYS	PRO	ALA	ASN	LEU	THR	ASP	ASN	ASN	CYS
GLN	ILE	ASP	LYS	E1789	LEU			ILE	PRO	SER	LYS	LEU	LYS	VAL	ILE	LYS	ASP	LEU
THR	SER	VAL	ALA		SER	R1441	T1253	ALA	VAL	LEU	ARG	LEU	PHE	ASN	LEU	ILE	PHE	MET
GLN	PRO	ASP	VAL	I1793	LYS	V1442	K1254	LYS	LYS	SER	PHE	LEU	TRP	LEU	PRO	ASP	TYR	ASN
VAL	PRO	SER	LYS		ILE			ALA	PRO	PRO	SER	ASN	GLU	LYS	GLY	LEU	PRO	SER
PRO	GLU	ASN	LYS	N1815	ILE	G1466	R1266	LYS	LEU	SER	ASN	VAL	SER	ASN	GLN	ARG	GLY	ALA
ALA	ILE	LYS	LYS		ASN	GLU		GLY	SER	LEU	LYS	LEU	CYS	ILE	LEU	SER	LEU	THR
ALA	SER	LYS	LYS	T1819	GLU	ARG	L1276	LYS	LYS	SER	LEU	GLU	TRP	ASN	SER	PHE	GLY	ALA
ILE	ASN	ALA	LYS	R1820	LEU	ASN		GLY	MET	SER	THR	THR	LEU	VAL	LYS	HIS	ALA	LEU
THR	ASN	ALA	GLU		G1530	TYR	E1292	ILE	GLU	THR	GLU	PHE	PHE	MET	ILE	ASP	ALA	LEU
LYS	GLU	ALA	LYS	H1830		GLU	R1293	GLN	LEU	ILE	GLN	LYS	LEU	LEU	LEU	GLY	SER	ARG



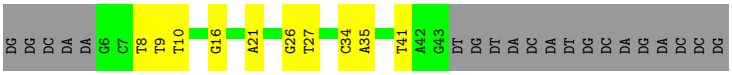
- Molecule 16: RNA

Chain P:



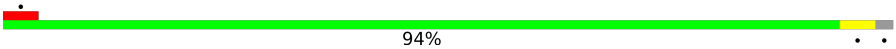
- Molecule 17: Template strand

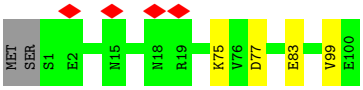
Chain T:



- Molecule 18: Transcription elongation factor SPT4

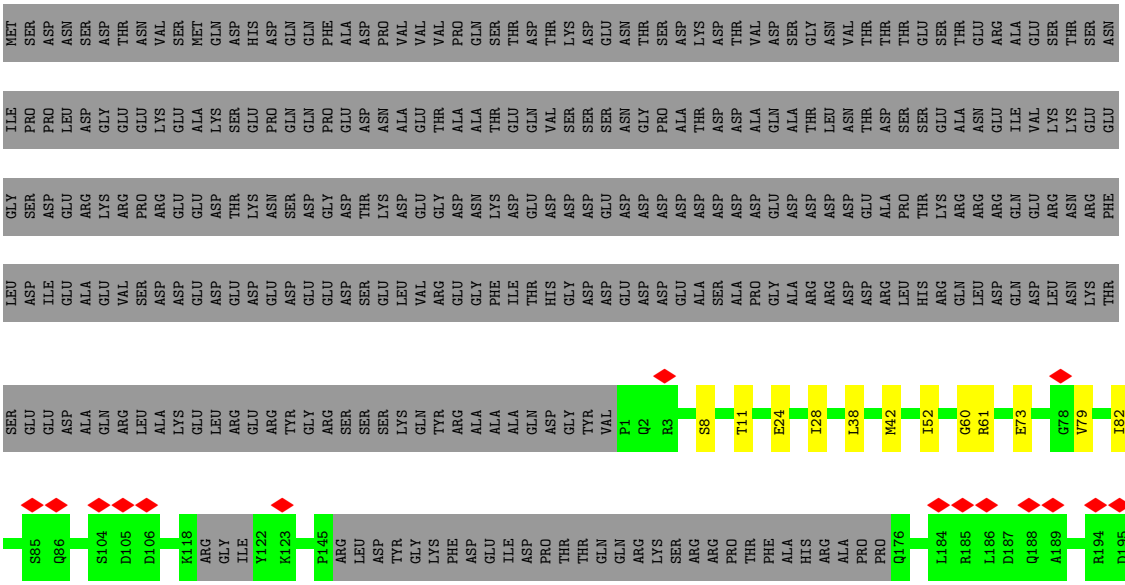
Chain Y:

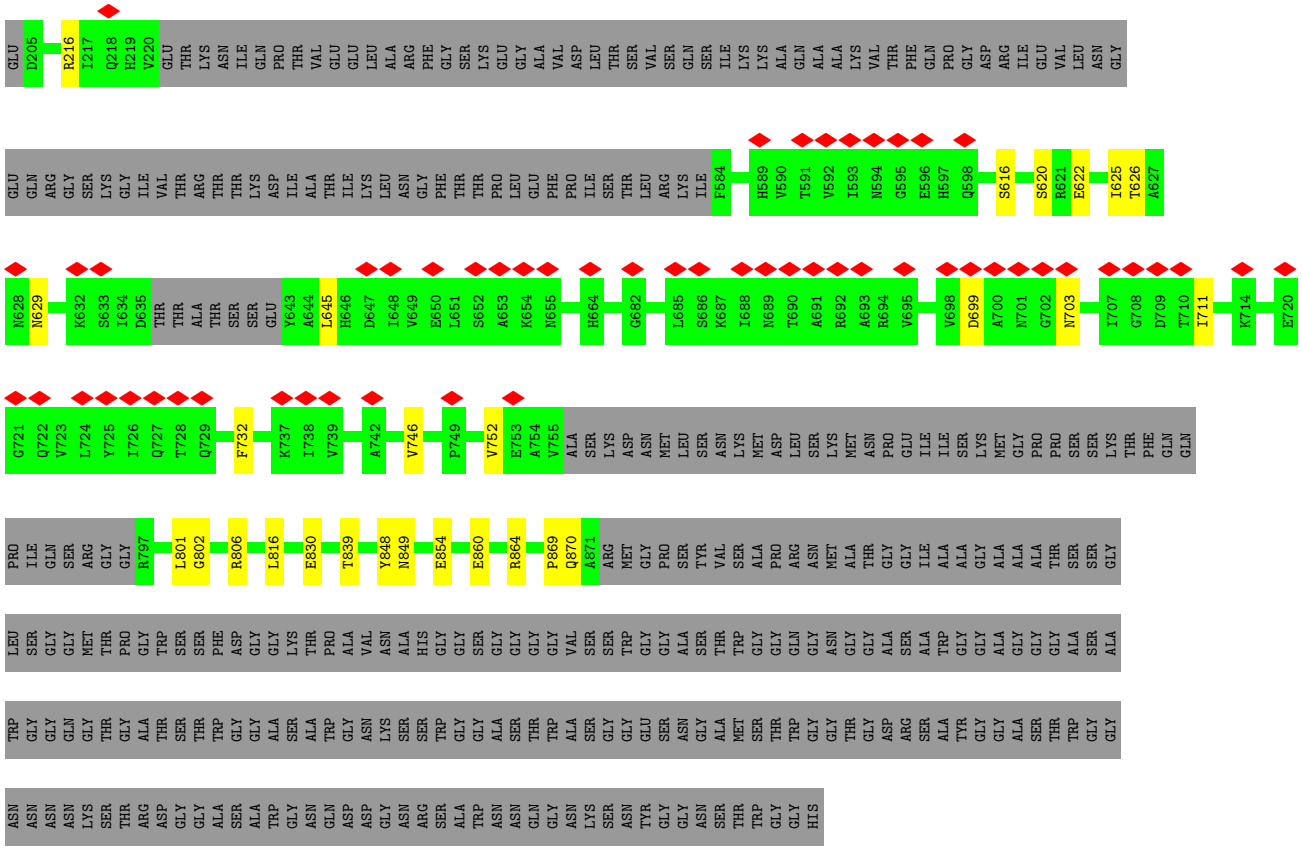




- Molecule 19: Transcription elongation factor SPT5

Chain Z:

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GLU GLN ARG GLY SER LYS GLY ILE VAL THR ARG THR THR LYS ASP ILE ALA THR ILE LYS LEU ASN GLY PHE THR THR PRO LEU GLU PHE PRO ILE SER THR LEU ARG LYS ILE F584 H589 V590 T591 V592 I593 N594 G595 E596 H597 Q598 S616 S620 R621 E622 I625 T626 A627
N628 N629 K632 S633 I634 D635 THR THR ALA THR SER SER GLU Y643 A644 L645 H646 D647 I648 V649 E650 L651 S652 A653 K654 N655 H664 G682 L685 S686 K687 I688 N689 T690 A691 R692 A693 R694 V695 V698 D699 A700 N701 G702 N703 I707 G708 D709 T710 I711 K714 E720
G721 Q722 V723 L724 Y725 I726 Q727 T728 Q729 F732 K737 I738 V739 A742 V746 P749 V752 E753 A754 V755 ALA SER LYS ASP ASN MET LEU SER ASN LYS MET ASP LEU SER LYS MET ASN PRO GLU ILE ILE SER LYS MET GLY PRO PRO SER SER LYS THR PHE GLN GLN
PRO ILE GLN SER ARG GLY GLY R797 L801 G802 R806 L816 E830 T839 Y848 N849 E854 E860 R864 P869 Q870 A871 ARG MET GLY PRO SER TYR VAL SER ALA PRO ARG ASN MET ALA THR GLY GLY ILE ALA ALA GLY ALA ALA ALA THR SER SER GLY
LEU SER GLY GLY MET THR PRO GLY TRP SER SER PHE ASP GLY GLY LYS THR PRO ALA VAL ASN ALA HIS GLY GLY SER GLY GLY GLY VAL SER SER TRP GLY GLY ALA SER THR TRP GLY GLY GLN GLY ASN GLY GLY GLY ALA SER ALA TRP GLY GLY ALA GLY GLY GLY ALA ALA SER SER ALA
TRP GLY GLY GLN GLY THR GLY ALA THR SER THR TRP GLY GLY ALA SER ALA TRP GLY ASN LYS SER SER TRP GLY GLY ALA SER THR TRP ALA SER GLY GLY GLU SER ASN GLY ALA MET SER THR TRP GLY GLY THR GLY ASP ARG SER ALA TYR GLY GLY ALA GLY GLY GLY SER THR TRP GLY GLY
ASN ASN ASN ASN LYS SER THR ARG ASP GLY GLY ALA SER ALA TRP GLY ASN GLN ASP ASP GLY ASN ARG SER ALA TRP ASN ASN GLN GLY ASN LYS SER ASN TYR GLY GLY ASN SER THR TRP GLY GLY HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9095	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 ($e^-/Å^2$)	40.02	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.042	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, ADP, MG, BEF

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	0.08	0/11217	0.21	0/15166
2	B	0.08	0/9011	0.22	0/12149
3	C	0.08	0/2116	0.20	0/2868
4	D	0.08	0/1279	0.19	0/1716
5	E	0.09	0/1788	0.21	0/2406
6	F	0.09	0/700	0.21	0/945
7	G	0.09	0/1368	0.20	0/1844
8	H	0.08	0/1086	0.24	0/1470
9	I	0.10	0/982	0.24	0/1321
10	J	0.11	0/541	0.22	0/727
11	K	0.10	0/938	0.19	0/1267
12	L	0.10	0/345	0.27	0/457
13	M	0.06	0/512	0.19	0/689
14	N	0.17	0/611	0.40	0/936
15	O	0.08	0/5659	0.20	0/7624
16	P	0.05	0/603	0.13	0/937
17	T	0.17	0/881	0.43	0/1360
18	Y	0.09	0/776	0.18	0/1050
19	Z	0.08	0/3419	0.21	0/4599
All	All	0.09	0/43832	0.22	0/59531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11020	0	11104	159	0
2	B	8839	0	8896	120	0
3	C	2078	0	2041	29	0
4	D	1270	0	1287	13	0
5	E	1752	0	1776	20	0
6	F	688	0	707	6	0
7	G	1340	0	1357	13	0
8	H	1068	0	1040	11	0
9	I	964	0	922	9	0
10	J	532	0	542	6	0
11	K	920	0	929	18	0
12	L	343	0	363	3	0
13	M	504	0	480	5	0
14	N	547	0	306	3	0
15	O	5557	0	5587	47	0
16	P	540	0	272	3	0
17	T	786	0	431	10	0
18	Y	760	0	741	3	0
19	Z	3374	0	3478	39	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
21	O	1	0	0	0	0
22	O	27	0	12	0	0
23	O	4	0	0	3	0
All	All	42924	0	42271	450	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 5.

All (450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:HIS:CD2	19:Z:645:LEU:HD22	1.57	1.38
2:B:1177:HIS:CD2	19:Z:645:LEU:CD2	2.21	1.22
2:B:1177:HIS:NE2	19:Z:645:LEU:HD22	1.58	1.18
2:B:1177:HIS:HD2	19:Z:645:LEU:CD2	1.78	0.96
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.53	0.89
1:A:853:ASP:OD1	1:A:855:THR:OG1	1.94	0.85
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.58	0.85
2:B:1177:HIS:CD2	19:Z:645:LEU:HD23	2.11	0.83
19:Z:849:ASN:ND2	19:Z:869:PRO:O	2.15	0.80
2:B:1177:HIS:NE2	19:Z:645:LEU:CD2	2.33	0.80
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.00	0.80
1:A:344:ARG:NH1	17:T:27:DT:OP1	2.15	0.79
4:D:22:GLU:OE1	4:D:28:GLN:NE2	2.15	0.79
1:A:811:GLN:NE2	2:B:705:MET:SD	2.56	0.78
1:A:885:THR:O	1:A:940:ARG:NH1	2.17	0.78
1:A:350:ARG:NH1	1:A:486:GLU:OE1	2.17	0.78
15:O:1654:GLN:NE2	15:O:1676:ASP:OD1	2.16	0.78
2:B:287:ARG:NH1	2:B:292:ILE:O	2.16	0.78
15:O:1191:VAL:O	15:O:1266:ARG:NH2	2.17	0.78
1:A:134:ARG:NH1	1:A:221:SER:O	2.17	0.77
15:O:1125:TYR:O	15:O:1173:ARG:NH1	2.18	0.77
2:B:906:SER:OG	19:Z:830:GLU:OE1	2.03	0.77
2:B:822:ASN:O	10:J:48:ARG:NH1	2.18	0.76
11:K:11:LEU:O	11:K:37:LYS:NZ	2.18	0.76
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.67	0.76
7:G:97:HIS:NE2	19:Z:622:GLU:OE2	2.19	0.75
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.21	0.74
13:M:37:THR:OG1	13:M:46:THR:OG1	2.05	0.74
2:B:315:LYS:NZ	2:B:319:GLU:OE2	2.19	0.74
7:G:25:TYR:O	7:G:28:THR:OG1	2.05	0.74
1:A:215:SER:OG	1:A:218:ASP:OD1	2.05	0.74
2:B:971:THR:OG1	3:C:61:GLU:OE1	2.03	0.74
1:A:567:LYS:NZ	8:H:93:TYR:O	2.21	0.73
2:B:101:MET:O	2:B:169:ARG:NH2	2.20	0.73
2:B:39:ARG:NH2	2:B:665:GLU:OE1	2.21	0.73
7:G:129:SER:OG	7:G:137:ILE:O	2.07	0.73
2:B:26:THR:OG1	2:B:29:ASP:OD1	2.06	0.72
19:Z:626:THR:OG1	19:Z:629:ASN:OD1	2.07	0.72
1:A:782:ARG:NH2	1:A:785:PRO:O	2.22	0.72
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.23	0.72
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.23	0.71
1:A:1100:ARG:NH2	1:A:1330:ASN:OD1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:SG	1:A:164:ARG:NH2	2.64	0.70
1:A:360:GLU:OE1	1:A:459:ARG:NH2	2.24	0.70
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.25	0.70
8:H:8:ASP:OD1	8:H:9:ILE:N	2.24	0.70
2:B:857:ARG:NH1	2:B:858:SER:O	2.25	0.70
2:B:98:THR:O	2:B:126:SER:OG	2.05	0.69
18:Y:75:LYS:NZ	18:Y:77:ASP:OD1	2.25	0.69
9:I:19:ASP:O	9:I:23:ASN:N	2.24	0.69
1:A:291:GLU:N	1:A:291:GLU:OE1	2.25	0.69
1:A:711:ARG:NH1	9:I:95:THR:O	2.26	0.69
1:A:291:GLU:OE2	19:Z:61:ARG:NH2	2.26	0.69
2:B:53:GLN:NE2	2:B:547:VAL:O	2.26	0.69
2:B:341:LEU:HD22	19:Z:73:GLU:OE1	1.93	0.69
1:A:1386:ARG:O	1:A:1391:ARG:NH1	2.26	0.68
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.27	0.68
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.27	0.68
4:D:139:LYS:O	4:D:143:ASN:ND2	2.27	0.68
4:D:153:ARG:NH2	4:D:182:SER:O	2.26	0.68
2:B:805:THR:OG1	2:B:1041:GLU:OE2	2.12	0.68
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.27	0.67
17:T:41:DT:OP2	19:Z:216:ARG:NH1	2.28	0.67
2:B:1177:HIS:NE2	19:Z:645:LEU:HB2	2.09	0.67
1:A:881:GLN:HB2	1:A:956:LEU:HD12	1.77	0.67
2:B:649:LYS:NZ	2:B:737:THR:O	2.27	0.67
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.27	0.67
1:A:951:GLU:OE1	1:A:953:ASN:N	2.28	0.66
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.13	0.66
1:A:114:LEU:O	1:A:164:ARG:NH1	2.29	0.66
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.29	0.66
3:C:226:ASP:OD1	3:C:227:THR:N	2.28	0.66
7:G:85:GLU:N	7:G:85:GLU:OE1	2.28	0.65
15:O:1668:GLU:O	15:O:1671:GLN:NE2	2.30	0.65
1:A:43:GLU:O	1:A:44:THR:OG1	2.14	0.65
2:B:328:GLU:N	2:B:328:GLU:OE1	2.30	0.65
8:H:3:ASN:OD1	8:H:4:THR:N	2.30	0.65
2:B:496:ARG:NH2	2:B:540:SER:O	2.29	0.64
2:B:711:GLU:N	2:B:711:GLU:OE1	2.29	0.64
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.30	0.64
1:A:1155:ASP:OD2	1:A:1239:ARG:NH2	2.31	0.64
15:O:1293:ARG:NH1	15:O:1570:SER:O	2.30	0.63
19:Z:28:ILE:CD1	19:Z:52:ILE:HG22	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.31	0.63
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.31	0.63
1:A:1390:ASN:OD1	1:A:1391:ARG:NH2	2.32	0.63
2:B:287:ARG:NE	2:B:324:ILE:O	2.31	0.63
3:C:4:GLU:OE2	11:K:104:ASN:ND2	2.31	0.62
2:B:995:ARG:NH2	11:K:39:ASP:OD2	2.32	0.62
2:B:125:SER:O	2:B:169:ARG:NH2	2.33	0.62
19:Z:38:LEU:HB3	19:Z:42:MET:HE2	1.80	0.62
2:B:776:GLN:OE1	16:P:33:A:O2'	2.15	0.62
2:B:868:MET:O	2:B:869:SER:OG	2.17	0.62
2:B:1177:HIS:HD2	19:Z:645:LEU:HD23	1.51	0.62
9:I:90:GLN:OE1	9:I:92:ARG:NH1	2.33	0.61
2:B:908:GLU:N	2:B:908:GLU:OE1	2.33	0.61
2:B:639:ILE:HD12	2:B:688:GLY:O	2.00	0.61
1:A:154:SER:OG	1:A:157:ASP:O	2.18	0.61
19:Z:854:GLU:N	19:Z:854:GLU:OE1	2.33	0.61
2:B:310:MET:HG3	2:B:386:LEU:HD13	1.83	0.61
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.34	0.61
1:A:1318:THR:HG23	5:E:141:VAL:HG11	1.83	0.61
19:Z:8:SER:HG	19:Z:11:THR:HG1	1.49	0.60
2:B:816:GLU:N	2:B:816:GLU:OE1	2.34	0.60
4:D:41:GLN:OE1	4:D:41:GLN:N	2.34	0.60
15:O:1127:ARG:NE	15:O:1129:SER:OG	2.34	0.60
1:A:1168:GLU:N	1:A:1168:GLU:OE1	2.35	0.60
2:B:499:ASN:OD1	2:B:500:THR:N	2.35	0.59
19:Z:860:GLU:N	19:Z:860:GLU:OE1	2.34	0.59
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.36	0.59
2:B:904:ARG:NH1	2:B:905:VAL:O	2.35	0.59
15:O:1699:PHE:O	15:O:1854:ALA:N	2.35	0.59
1:A:22:PHE:CE2	1:A:27:VAL:HG22	2.38	0.59
2:B:733:HIS:O	2:B:733:HIS:ND1	2.35	0.59
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.02	0.59
4:D:150:ASN:OD1	4:D:151:PHE:N	2.36	0.59
5:E:40:GLU:OE1	5:E:43:LYS:NZ	2.35	0.59
2:B:399:ASP:OD2	2:B:510:LYS:NZ	2.35	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.85	0.58
2:B:262:GLU:OE1	2:B:267:ARG:NH2	2.36	0.58
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.34	0.58
3:C:90:ASP:OD1	19:Z:848:TYR:OH	2.22	0.58
1:A:173:THR:OG1	1:A:184:SER:OG	2.22	0.58
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:O	1:A:273:ASN:ND2	2.36	0.58
19:Z:870:GLN:OE1	19:Z:870:GLN:N	2.36	0.58
5:E:36:GLU:OE1	5:E:36:GLU:N	2.37	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.57
1:A:871:ASP:OD1	5:E:204:THR:OG1	2.18	0.57
2:B:567:GLU:N	2:B:567:GLU:OE1	2.38	0.57
1:A:43:GLU:OE1	1:A:43:GLU:N	2.36	0.57
1:A:68:GLN:N	1:A:68:GLN:OE1	2.38	0.57
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.37	0.57
2:B:570:VAL:O	2:B:570:VAL:HG13	2.04	0.57
15:O:1770:MET:N	15:O:1770:MET:SD	2.78	0.57
1:A:293:GLU:OE2	1:A:297:GLN:NE2	2.39	0.56
1:A:808:LEU:O	2:B:728:ARG:NH2	2.39	0.56
2:B:1129:ARG:NE	17:T:26:DG:OP1	2.35	0.56
5:E:33:GLU:N	5:E:33:GLU:OE1	2.38	0.56
11:K:36:GLU:OE1	11:K:70:ARG:NE	2.38	0.56
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.38	0.56
1:A:205:GLU:N	1:A:205:GLU:OE1	2.38	0.56
7:G:117:GLN:N	7:G:117:GLN:OE1	2.39	0.56
4:D:199:ASN:OD1	4:D:200:ASN:N	2.35	0.56
1:A:588:LEU:HD23	1:A:589:GLN:N	2.21	0.56
1:A:917:SER:OG	1:A:918:GLU:OE1	2.21	0.56
13:M:39:ASP:O	13:M:43:SER:N	2.39	0.56
5:E:85:GLU:N	5:E:85:GLU:OE1	2.38	0.56
1:A:365:GLY:N	1:A:469:ARG:O	2.34	0.56
1:A:660:ASN:O	2:B:1082:MET:N	2.39	0.56
15:O:1591:GLU:OE2	23:O:3003:BEF:F1	2.14	0.56
1:A:1169:ILE:HG21	1:A:1239:ARG:HD3	1.87	0.56
15:O:1246:LYS:NZ	15:O:1292:GLU:OE2	2.20	0.55
11:K:64:GLU:OE1	11:K:64:GLU:N	2.39	0.55
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.36	0.55
2:B:357:GLN:NE2	2:B:368:GLU:OE1	2.39	0.55
1:A:451:HIS:NE2	1:A:477:PRO:O	2.36	0.55
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.87	0.55
2:B:468:GLU:N	2:B:468:GLU:OE1	2.38	0.55
11:K:79:GLU:OE1	11:K:79:GLU:N	2.38	0.55
2:B:1177:HIS:NE2	19:Z:645:LEU:CB	2.69	0.55
15:O:1253:THR:HG22	15:O:1254:LYS:H	1.71	0.55
1:A:67:CYS:O	1:A:71:GLN:N	2.39	0.55
4:D:157:GLN:N	4:D:157:GLN:OE1	2.40	0.54
1:A:344:ARG:NE	2:B:1120:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD11	2:B:658:ILE:HG13	1.88	0.54
2:B:872:GLU:N	2:B:872:GLU:OE1	2.38	0.54
2:B:996:ARG:CZ	3:C:38:ILE:HD11	2.37	0.54
1:A:1223:ASP:C	1:A:1224:LEU:HD12	2.33	0.54
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.89	0.54
2:B:610:ASN:O	2:B:613:VAL:HG12	2.08	0.54
3:C:215:GLU:OE1	3:C:215:GLU:N	2.40	0.54
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.40	0.54
7:G:22:MET:SD	7:G:23:LYS:N	2.81	0.54
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.89	0.53
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.90	0.53
5:E:185:ALA:O	5:E:189:GLY:N	2.40	0.53
18:Y:99:VAL:HG12	18:Y:99:VAL:O	2.09	0.53
11:K:38:GLU:OE1	11:K:42:LEU:HD12	2.08	0.53
15:O:1431:GLN:OE1	15:O:1431:GLN:N	2.39	0.53
1:A:577:ILE:O	1:A:580:VAL:HG22	2.08	0.53
18:Y:83:GLU:OE1	18:Y:83:GLU:N	2.39	0.53
19:Z:24:GLU:OE1	19:Z:24:GLU:N	2.40	0.53
15:O:1776:ASP:OD1	15:O:1777:PHE:N	2.41	0.53
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.44	0.53
15:O:1191:VAL:HG23	15:O:1194:PHE:HB2	1.90	0.53
1:A:593:GLU:OE1	1:A:593:GLU:N	2.41	0.53
8:H:106:GLU:OE1	8:H:106:GLU:N	2.41	0.53
1:A:348:SER:HB2	2:B:1128:LEU:HD22	1.91	0.52
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.25	0.52
2:B:760:ASP:OD1	2:B:761:HIS:ND1	2.42	0.52
3:C:11:ARG:NH1	3:C:12:GLU:OE2	2.42	0.52
2:B:322:PHE:O	2:B:325:GLN:NE2	2.40	0.52
1:A:1189:SER:O	1:A:1241:ARG:NH1	2.41	0.52
3:C:259:LEU:HD21	11:K:91:CYS:HB2	1.91	0.52
5:E:90:VAL:HG23	14:N:51:DA:OP1	2.08	0.52
2:B:564:GLU:N	2:B:564:GLU:OE1	2.40	0.52
15:O:1707:GLN:N	15:O:1707:GLN:OE1	2.42	0.52
2:B:762:ASN:OD1	2:B:763:GLN:N	2.42	0.52
5:E:168:TYR:HB3	5:E:170:LEU:HD13	1.91	0.52
15:O:1820:ARG:NH2	23:O:3003:BEF:F3	2.32	0.52
1:A:863:VAL:O	1:A:863:VAL:HG23	2.10	0.52
3:C:58:LEU:HD11	10:J:2:ILE:HD11	1.92	0.52
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.27	0.52
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.52
1:A:1211:GLN:OE1	1:A:1274:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ILE:HD11	7:G:29:LYS:HD3	1.92	0.51
2:B:1174:LYS:O	2:B:1178:ASN:N	2.43	0.51
5:E:138:ALA:O	5:E:141:VAL:HG12	2.09	0.51
1:A:790:ASP:OD2	9:I:87:GLN:N	2.43	0.51
1:A:1412:ALA:O	1:A:1416:ALA:N	2.44	0.51
3:C:111:THR:HG23	15:O:1266:ARG:HH22	1.76	0.51
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.51
15:O:1619:GLN:NE2	23:O:3003:BEF:F3	2.34	0.51
3:C:47:ASP:OD1	12:L:70:ARG:NH1	2.44	0.51
1:A:394:ASN:ND2	1:A:400:PRO:O	2.41	0.50
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.42	0.50
5:E:48:ASP:OD1	5:E:51:GLY:N	2.44	0.50
3:C:17:ASN:OD1	3:C:231:ASN:ND2	2.42	0.50
19:Z:801:LEU:HD23	19:Z:802:GLY:N	2.26	0.50
1:A:874:ASP:N	1:A:1056:SER:O	2.38	0.50
1:A:101:LYS:NZ	14:N:43:DC:OP1	2.37	0.50
1:A:526:ASP:OD2	2:B:835:GLN:NE2	2.44	0.50
2:B:786:ASN:O	2:B:967:ARG:NH2	2.45	0.50
1:A:406:ILE:N	1:A:431:LYS:O	2.45	0.50
19:Z:24:GLU:OE2	19:Z:60:GLY:N	2.39	0.50
1:A:845:LEU:HD23	1:A:848:ILE:HD12	1.94	0.50
1:A:1324:PRO:O	1:A:1327:ILE:HG22	2.12	0.50
7:G:11:ILE:HD13	7:G:26:LEU:HG	1.94	0.50
14:N:45:DT:O2	17:T:16:DG:N2	2.45	0.50
19:Z:711:ILE:HD12	19:Z:711:ILE:C	2.36	0.50
2:B:120:ARG:NH2	2:B:956:THR:O	2.45	0.50
2:B:1035:ALA:O	2:B:1039:GLY:N	2.44	0.50
15:O:1183:ILE:HG22	15:O:1201:VAL:HG22	1.94	0.50
2:B:766:ARG:NH2	2:B:985:GLY:O	2.45	0.49
9:I:60:GLN:OE1	9:I:60:GLN:N	2.41	0.49
15:O:1332:SER:OG	15:O:1430:LYS:O	2.16	0.49
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.47	0.49
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.93	0.49
1:A:544:ASP:O	11:K:47:ARG:NH2	2.45	0.49
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.44	0.49
15:O:1441:ARG:NH1	15:O:1442:VAL:O	2.45	0.49
8:H:92:ASP:O	8:H:145:ARG:NH2	2.45	0.49
19:Z:732:PHE:CD1	19:Z:746:VAL:HG22	2.48	0.49
4:D:34:GLN:N	4:D:34:GLN:OE1	2.46	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.53	0.49
15:O:1127:ARG:NH2	15:O:1134:ASP:OD1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.43	0.49
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.45	0.49
3:C:258:ILE:HD11	11:K:42:LEU:HD13	1.93	0.49
9:I:68:LEU:O	9:I:70:ARG:NH1	2.45	0.49
1:A:23:SER:O	1:A:27:VAL:HG23	2.12	0.49
1:A:443:LEU:CD1	1:A:455:MET:HE2	2.39	0.49
1:A:1042:PHE:CE1	1:A:1046:LEU:HD11	2.48	0.49
1:A:782:ARG:NE	1:A:787:PHE:O	2.42	0.48
17:T:35:DA:H2'	17:T:35:DA:N3	2.28	0.48
2:B:481:GLN:NE2	16:P:32:C:OP1	2.47	0.48
1:A:349:ALA:O	2:B:1128:LEU:HD21	2.13	0.48
2:B:364:ILE:CD1	2:B:365:THR:HG22	2.44	0.48
1:A:74:MET:O	2:B:1116:ARG:NH1	2.47	0.48
1:A:334:GLY:O	1:A:338:GLY:N	2.46	0.48
15:O:1702:ILE:O	15:O:1830:HIS:ND1	2.45	0.48
1:A:1216:ILE:HG21	1:A:1226:VAL:HG21	1.96	0.48
2:B:618:ASP:O	2:B:622:LYS:N	2.47	0.48
2:B:1176:ASN:OD1	2:B:1177:HIS:CD2	2.67	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.44	0.48
2:B:824:ILE:N	2:B:824:ILE:HD12	2.28	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:CG2	2.43	0.48
2:B:566:LEU:HD22	2:B:586:TRP:O	2.14	0.48
17:T:8:DT:H2'	17:T:9:DT:H71	1.96	0.47
19:Z:28:ILE:HD13	19:Z:52:ILE:HG22	1.95	0.47
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.97	0.47
15:O:1339:GLN:NE2	15:O:1361:THR:O	2.46	0.47
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.95	0.47
11:K:37:LYS:N	11:K:69:ALA:O	2.46	0.47
15:O:1408:ILE:HD12	15:O:1408:ILE:N	2.30	0.47
1:A:894:GLU:OE2	1:A:933:TYR:OH	2.30	0.47
3:C:38:ILE:HB	3:C:176:ILE:HD12	1.97	0.47
1:A:475:THR:O	1:A:479:ASN:N	2.47	0.47
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.45	0.47
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.97	0.47
15:O:1731:TYR:OH	15:O:1735:LYS:NZ	2.32	0.47
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.96	0.47
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.47
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.96	0.47
1:A:247:ARG:NH2	1:A:263:THR:OG1	2.43	0.46
1:A:557:ASP:OD1	1:A:558:GLY:N	2.46	0.46
2:B:640:VAL:HG12	2:B:649:LYS:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1362:GLY:O	15:O:1366:THR:N	2.43	0.46
19:Z:699:ASP:OD1	19:Z:703:ASN:N	2.49	0.46
1:A:1234:GLU:OE1	1:A:1234:GLU:N	2.40	0.46
2:B:364:ILE:HD12	2:B:365:THR:HG22	1.96	0.46
2:B:806:THR:HG23	2:B:1045:SER:HA	1.96	0.46
8:H:40:LEU:HD21	8:H:42:ILE:HD11	1.97	0.46
4:D:133:THR:O	4:D:134:THR:OG1	2.30	0.46
15:O:1641:ARG:O	15:O:1645:ASN:ND2	2.43	0.46
15:O:1749:ILE:HD11	15:O:1793:ILE:HG12	1.96	0.46
6:F:79:ARG:NH1	6:F:145:ASP:O	2.49	0.46
1:A:356:ASP:OD1	11:K:65:HIS:NE2	2.47	0.46
1:A:68:GLN:O	1:A:71:GLN:NE2	2.49	0.46
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.16	0.46
19:Z:860:GLU:O	19:Z:864:ARG:N	2.45	0.46
3:C:101:LEU:HD23	3:C:102:GLN:N	2.31	0.45
1:A:830:LYS:O	1:A:834:THR:HG23	2.17	0.45
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.46	0.45
9:I:21:GLU:OE1	9:I:21:GLU:N	2.45	0.45
1:A:457:ALA:O	1:A:507:VAL:HG23	2.17	0.45
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.38	0.45
6:F:85:MET:HE2	6:F:90:ARG:HA	1.98	0.45
15:O:1309:GLN:O	15:O:1313:ALA:N	2.50	0.45
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.99	0.45
1:A:453:MET:SD	1:A:453:MET:N	2.90	0.45
1:A:709:THR:HG23	1:A:712:GLU:H	1.82	0.45
2:B:773:MET:SD	2:B:987:LYS:NZ	2.81	0.45
3:C:234:SER:OG	3:C:238:ILE:O	2.12	0.45
7:G:39:THR:O	7:G:43:GLY:N	2.50	0.45
1:A:1450:LEU:HD23	1:A:1450:LEU:O	2.17	0.45
2:B:120:ARG:HE	2:B:122:LEU:HD11	1.81	0.45
2:B:326:ASP:OD1	2:B:327:ARG:N	2.50	0.45
2:B:337:ARG:NH1	13:M:65:GLN:OE1	2.50	0.45
1:A:1147:THR:HG22	1:A:1197:LEU:CD2	2.47	0.45
1:A:1318:THR:CG2	5:E:141:VAL:HG11	2.47	0.44
2:B:22:SER:O	2:B:654:ARG:NH1	2.50	0.44
3:C:111:THR:HG23	15:O:1266:ARG:NH2	2.32	0.44
15:O:1354:LEU:HD21	15:O:1642:MET:HB2	1.99	0.44
1:A:445:ASN:ND2	1:A:454:SER:O	2.51	0.44
2:B:417:PHE:O	2:B:418:LYS:C	2.59	0.44
4:D:45:GLU:OE1	4:D:45:GLU:N	2.49	0.44
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1167:GLN:NE2	16:P:2:G:O6	2.50	0.44
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.82	0.44
1:A:1386:ARG:NH2	17:T:21:DA:N3	2.65	0.44
12:L:40:LEU:HD21	12:L:56:LEU:HD21	1.98	0.44
15:O:1212:SER:HG	15:O:1215:ASP:CG	2.26	0.44
2:B:619:ILE:N	2:B:619:ILE:HD12	2.32	0.44
8:H:143:LEU:N	8:H:143:LEU:HD12	2.32	0.44
19:Z:616:SER:O	19:Z:620:SER:N	2.49	0.44
11:K:60:ALA:O	11:K:73:LEU:HD12	2.17	0.44
15:O:1315:PRO:HG3	15:O:1642:MET:HE3	2.00	0.44
2:B:310:MET:CG	2:B:386:LEU:HD13	2.48	0.44
3:C:36:VAL:HG13	11:K:41:THR:HG21	1.99	0.44
15:O:1137:ILE:N	15:O:1137:ILE:HD12	2.33	0.44
15:O:1733:PHE:O	15:O:1737:ASP:N	2.51	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.82	0.44
3:C:37:MET:SD	3:C:244:VAL:HG12	2.57	0.44
1:A:526:ASP:OD1	1:A:527:THR:N	2.50	0.44
2:B:228:LYS:O	2:B:261:ARG:NH1	2.51	0.44
15:O:1686:ARG:NE	15:O:1789:GLU:OE2	2.45	0.44
2:B:255:GLN:N	2:B:255:GLN:OE1	2.50	0.44
3:C:121:VAL:HA	15:O:1276:LEU:HD12	1.99	0.44
1:A:471:ASN:O	1:A:474:VAL:HG22	2.18	0.43
2:B:183:GLU:N	2:B:183:GLU:OE1	2.51	0.43
2:B:785:TYR:O	2:B:967:ARG:NH1	2.50	0.43
1:A:118:HIS:O	1:A:123:ARG:NH1	2.51	0.43
1:A:352:VAL:HG12	1:A:353:ILE:N	2.33	0.43
1:A:834:THR:HG21	1:A:1076:ALA:O	2.18	0.43
15:O:1779:THR:O	15:O:1783:PHE:N	2.50	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
13:M:34:VAL:HG13	13:M:47:LEU:HD21	2.00	0.43
17:T:9:DT:H2'	17:T:10:DT:H71	2.01	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
11:K:49:GLU:OE2	11:K:93:SER:OG	2.35	0.43
12:L:66:GLN:HE21	19:Z:816:LEU:HG	1.84	0.43
1:A:718:VAL:HG11	1:A:774:ARG:NH1	2.33	0.43
1:A:465:TYR:HB3	2:B:976:ILE:HD11	2.00	0.43
1:A:523:ILE:HG22	1:A:524:VAL:N	2.34	0.43
1:A:1169:ILE:HG21	1:A:1239:ARG:CD	2.49	0.43
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.43	0.43
8:H:38:LEU:C	8:H:38:LEU:HD23	2.44	0.43
2:B:581:PHE:O	2:B:626:ILE:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ARG:O	2:B:331:LEU:HD23	2.18	0.42
19:Z:625:ILE:HG22	19:Z:626:THR:N	2.35	0.42
1:A:225:ASN:O	1:A:229:SER:OG	2.33	0.42
1:A:715:GLU:OE1	1:A:774:ARG:NE	2.51	0.42
1:A:759:ALA:O	1:A:764:CYS:N	2.41	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.54	0.42
1:A:117:GLU:O	1:A:123:ARG:NH1	2.50	0.42
2:B:301:ILE:HD12	2:B:382:ILE:HG21	2.00	0.42
13:M:47:LEU:C	13:M:47:LEU:HD23	2.45	0.42
1:A:301:ALA:O	1:A:305:ASP:N	2.41	0.42
1:A:609:ASP:OD2	1:A:969:GLN:NE2	2.52	0.42
1:A:1209:MET:HE3	1:A:1236:LEU:HB3	2.00	0.42
3:C:35:ARG:NE	11:K:41:THR:OG1	2.42	0.42
4:D:192:LYS:NZ	4:D:199:ASN:O	2.50	0.42
8:H:35:GLN:OE1	8:H:35:GLN:N	2.41	0.42
15:O:1815:ASN:O	15:O:1819:THR:HG23	2.20	0.42
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.47	0.42
4:D:130:LEU:O	4:D:130:LEU:HD23	2.19	0.42
7:G:12:THR:OG1	7:G:69:GLU:OE1	2.20	0.42
19:Z:79:VAL:HG11	19:Z:82:ILE:HD12	2.01	0.42
1:A:543:LEU:HD13	1:A:572:TRP:CH2	2.54	0.42
9:I:54:GLU:OE2	9:I:118:ARG:NH2	2.52	0.42
1:A:199:LEU:N	1:A:199:LEU:HD12	2.35	0.42
15:O:1843:LEU:C	15:O:1843:LEU:HD23	2.45	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG21	2.01	0.42
6:F:130:ILE:HG22	6:F:132:LEU:H	1.85	0.42
3:C:260:LEU:HD23	3:C:260:LEU:O	2.20	0.41
5:E:165:LEU:O	5:E:169:ARG:N	2.52	0.41
15:O:1169:LEU:C	15:O:1169:LEU:HD23	2.45	0.41
1:A:181:LEU:HD12	1:A:181:LEU:O	2.20	0.41
7:G:119:LEU:HD23	7:G:120:THR:N	2.35	0.41
17:T:8:DT:C2'	17:T:9:DT:H71	2.49	0.41
1:A:658:LEU:HD23	1:A:658:LEU:O	2.19	0.41
1:A:1373:ASP:O	1:A:1377:THR:N	2.54	0.41
2:B:90:ILE:N	2:B:90:ILE:HD12	2.36	0.41
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.54	0.41
3:C:53:THR:OG1	3:C:154:LYS:NZ	2.53	0.41
15:O:1187:ASN:OD1	15:O:1188:ARG:N	2.54	0.41
17:T:34:DC:H4'	17:T:35:DA:H5'	2.02	0.41
1:A:35:ILE:HD12	1:A:35:ILE:N	2.35	0.41
1:A:64:ASN:C	1:A:65:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:229:SER:N	2.53	0.41
1:A:826:ASP:O	1:A:830:LYS:HG2	2.21	0.41
1:A:1259:MET:HE2	1:A:1259:MET:HA	2.01	0.41
2:B:269:ILE:HD12	2:B:269:ILE:N	2.35	0.41
2:B:845:SER:HB3	2:B:850:LEU:HD22	2.03	0.41
1:A:534:LEU:HD11	1:A:541:ILE:HD11	2.02	0.41
1:A:561:PRO:O	1:A:572:TRP:NE1	2.42	0.41
1:A:1121:GLU:O	1:A:1125:ALA:N	2.54	0.41
2:B:952:VAL:HG23	2:B:966:VAL:HG22	2.02	0.41
5:E:68:SER:O	5:E:72:PHE:N	2.45	0.41
5:E:50:MET:SD	5:E:52:ARG:NH2	2.91	0.41
7:G:103:VAL:O	7:G:103:VAL:HG13	2.19	0.41
19:Z:8:SER:OG	19:Z:11:THR:OG1	2.20	0.41
1:A:489:LEU:HD23	1:A:489:LEU:C	2.45	0.41
1:A:902:LEU:HD23	1:A:902:LEU:O	2.21	0.41
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.21	0.41
3:C:155:LEU:HD12	3:C:155:LEU:C	2.45	0.41
4:D:27:LEU:N	4:D:27:LEU:HD22	2.36	0.41
9:I:19:ASP:O	9:I:23:ASN:CA	2.69	0.41
1:A:349:ALA:C	2:B:1128:LEU:HD21	2.45	0.41
2:B:861:ASP:OD1	2:B:862:GLN:N	2.53	0.41
5:E:128:PRO:N	5:E:129:PRO:HD2	2.35	0.41
15:O:1216:LEU:HD12	15:O:1245:ALA:O	2.21	0.41
15:O:1574:HIS:ND1	15:O:1576:VAL:HG12	2.35	0.41
1:A:866:PHE:N	5:E:208:TYR:OH	2.53	0.40
1:A:1006:ILE:N	1:A:1006:ILE:HD12	2.36	0.40
1:A:1348:LEU:O	1:A:1348:LEU:HD23	2.21	0.40
2:B:1168:LEU:HD11	2:B:1208:MET:SD	2.61	0.40
3:C:33:LEU:HD13	3:C:248:ILE:CD1	2.50	0.40
1:A:34:LYS:C	1:A:35:ILE:HD12	2.46	0.40
19:Z:711:ILE:HD13	19:Z:752:VAL:CG1	2.51	0.40
1:A:399:HIS:O	1:A:435:HIS:ND1	2.53	0.40
1:A:397:ASN:HB3	19:Z:839:THR:HG21	2.02	0.40
1:A:1318:THR:O	1:A:1318:THR:HG22	2.20	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.44	0.40
19:Z:806:ARG:CZ	19:Z:816:LEU:HD21	2.51	0.40
1:A:1002:GLY:N	1:A:1007:ILE:HG21	2.37	0.40
3:C:260:LEU:HD23	3:C:260:LEU:C	2.47	0.40
15:O:1253:THR:HG22	15:O:1254:LYS:N	2.34	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	1388/1733 (80%)	1345 (97%)	43 (3%)	0	100	100
2	B	1099/1224 (90%)	1077 (98%)	22 (2%)	0	100	100
3	C	262/318 (82%)	251 (96%)	11 (4%)	0	100	100
4	D	155/221 (70%)	153 (99%)	2 (1%)	0	100	100
5	E	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
6	F	83/155 (54%)	82 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	169 (100%)	0	0	100	100
8	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
9	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	63 (100%)	0	0	100	100
11	K	113/120 (94%)	113 (100%)	0	0	100	100
12	L	41/70 (59%)	41 (100%)	0	0	100	100
13	M	63/145 (43%)	63 (100%)	0	0	100	100
15	O	688/2231 (31%)	675 (98%)	13 (2%)	0	100	100
18	Y	98/102 (96%)	98 (100%)	0	0	100	100
19	Z	412/1063 (39%)	406 (98%)	6 (2%)	0	100	100
All	All	5091/8106 (63%)	4981 (98%)	110 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1520 (81%)	1225 (100%)	0	100	100
2	B	964/1061 (91%)	964 (100%)	0	100	100
3	C	232/274 (85%)	231 (100%)	1 (0%)	84	82
4	D	141/200 (70%)	141 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	112/116 (97%)	112 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	60/131 (46%)	60 (100%)	0	100	100
15	O	618/2010 (31%)	618 (100%)	0	100	100
18	Y	85/87 (98%)	85 (100%)	0	100	100
19	Z	374/876 (43%)	374 (100%)	0	100	100
All	All	4548/7113 (64%)	4547 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
3	C	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	169	ASN
1	A	576	GLN
1	A	953	ASN
1	A	1059	HIS
2	B	52	ASN
2	B	481	GLN
2	B	538	ASN
2	B	951	GLN
3	C	151	GLN

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Mol	Chain	Res	Type
4	D	23	ASN
4	D	37	GLN
7	G	57	GLN
7	G	71	ASN
13	M	29	ASN
13	M	42	ASN
15	O	1241	HIS
15	O	1267	ASN
15	O	1738	ASN
19	Z	102	ASN
19	Z	835	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	23/35 (65%)	8 (34%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	3	U
16	P	4	C
16	P	5	G
16	P	6	U
16	P	9	G
16	P	21	G
16	P	23	G
16	P	25	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	ADP	O	3001	21	27,29,29	1.38	4 (14%)	42,45,45	2.05	12 (28%)
23	BEF	O	3003	-	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	O	3001	21	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	3001	ADP	C5-C4	4.59	1.47	1.39
22	O	3001	ADP	C5-C6	2.80	1.48	1.41
22	O	3001	ADP	C8-N7	2.55	1.36	1.31
22	O	3001	ADP	C5-N7	-2.20	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	3001	ADP	C5-C4-N3	-6.38	118.42	126.75
22	O	3001	ADP	N3-C4-N9	4.85	135.08	127.08
22	O	3001	ADP	C2-N3-C4	4.11	121.47	111.75
22	O	3001	ADP	PA-O3A-PB	-3.89	119.48	132.83
22	O	3001	ADP	N3-C2-N1	-3.58	123.00	128.60
22	O	3001	ADP	C4-C5-N7	-3.47	106.39	110.62
22	O	3001	ADP	C5-N7-C8	3.05	107.84	103.51
22	O	3001	ADP	C3'-C2'-C1'	2.56	106.28	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	3001	ADP	C4-N9-C8	2.45	108.39	105.73
22	O	3001	ADP	C6-C5-N7	2.29	136.28	132.02
22	O	3001	ADP	N9-C8-N7	-2.22	110.88	113.91
22	O	3001	ADP	C2-N1-C6	2.01	122.22	118.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

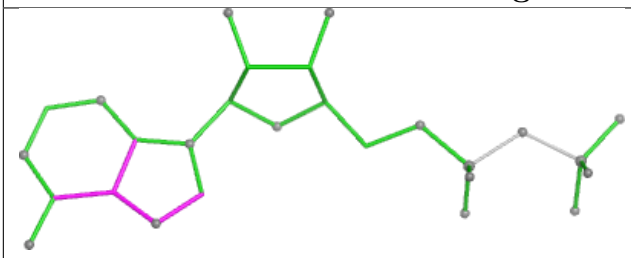
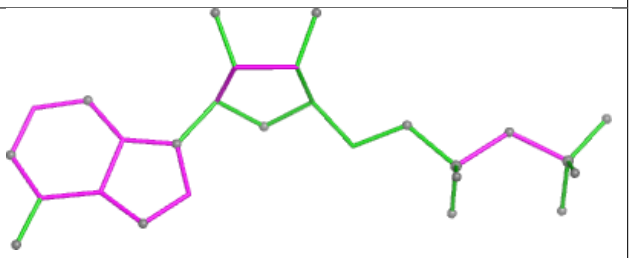
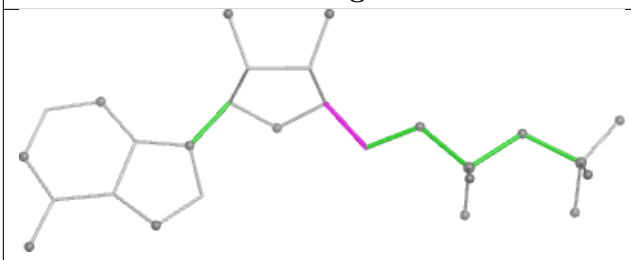
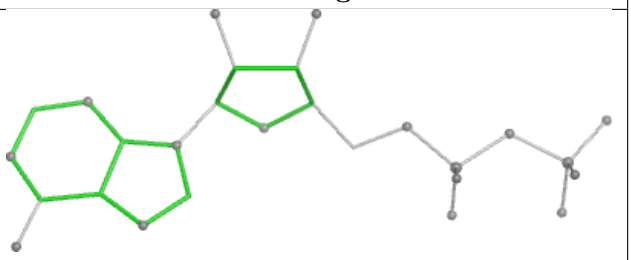
Mol	Chain	Res	Type	Atoms
22	O	3001	ADP	O4'-C4'-C5'-O5'
22	O	3001	ADP	C3'-C4'-C5'-O5'

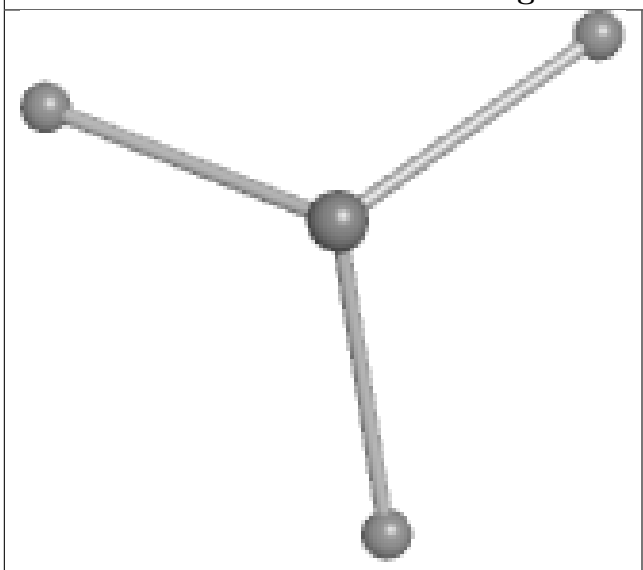
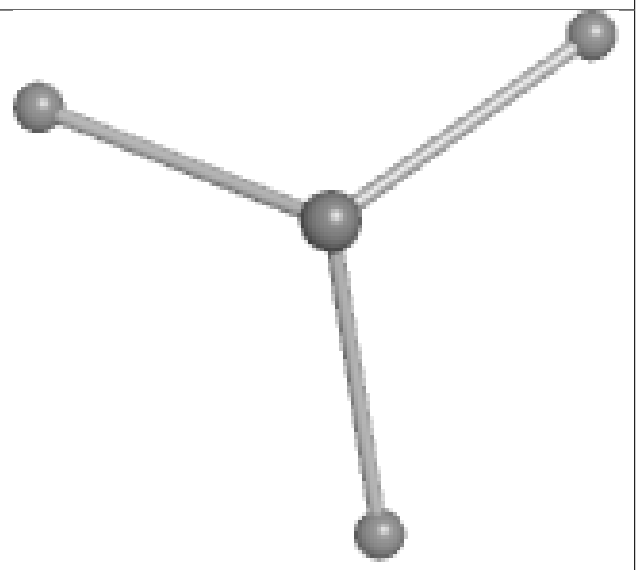
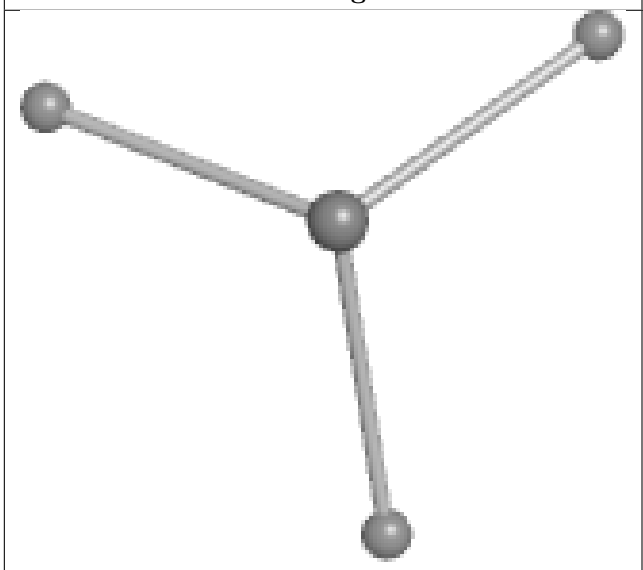
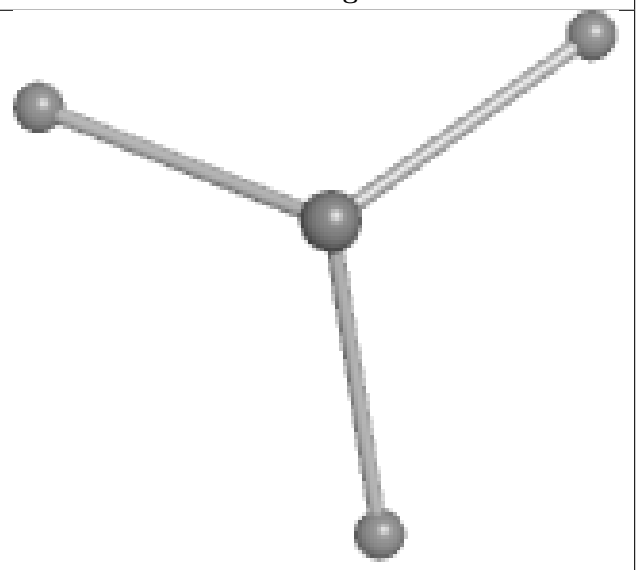
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	3003	BEF	3	0

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

Ligand ADP O 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BEF O 3003	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

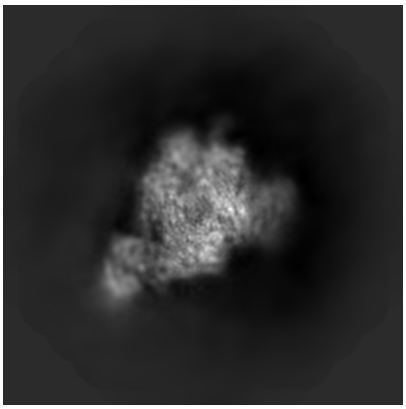
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19022. These allow visual inspection of the internal detail of the map and identification of artifacts.

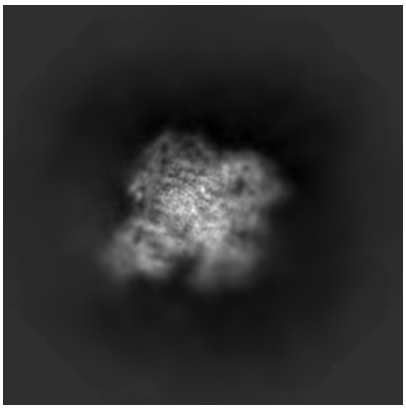
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

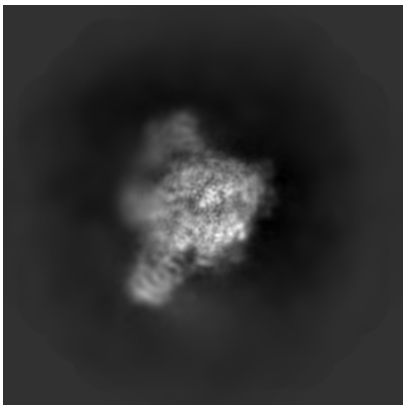
6.1.1 Primary map



X

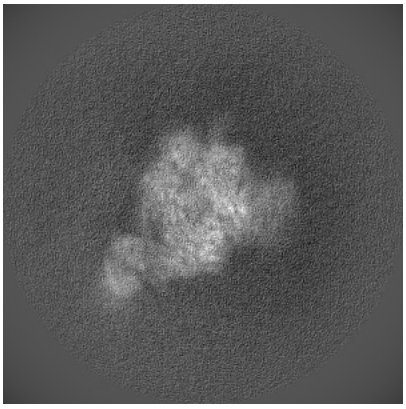


Y

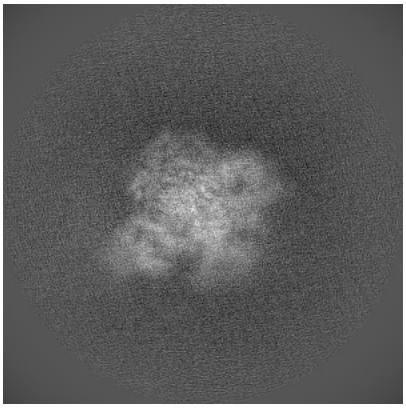


Z

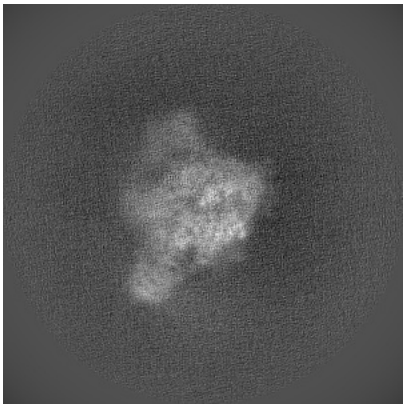
6.1.2 Raw map



X



Y

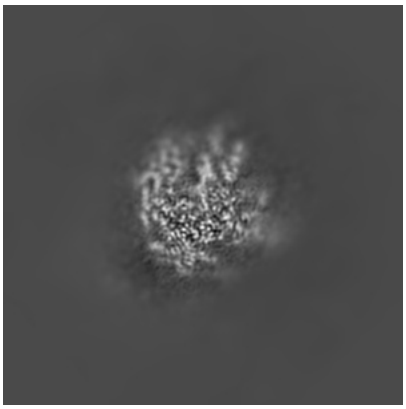


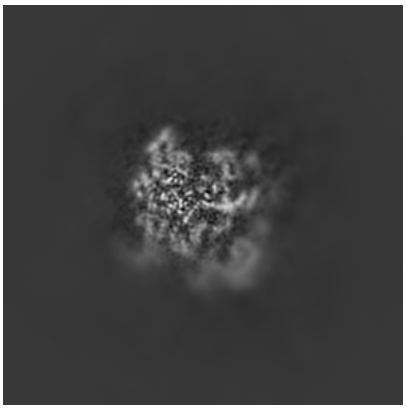
Z

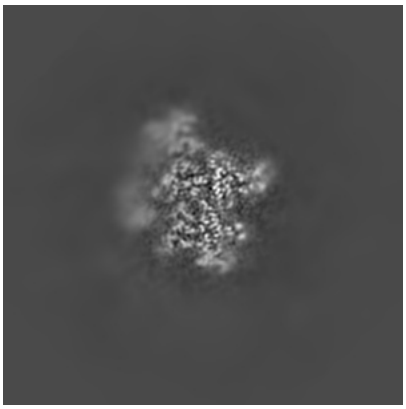
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

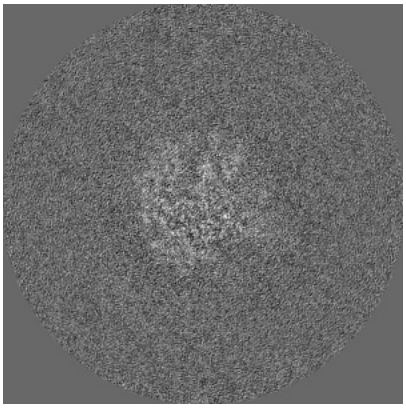
6.2.1 Primary map

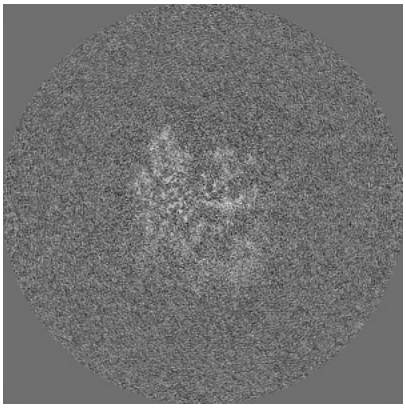

X Index: 180

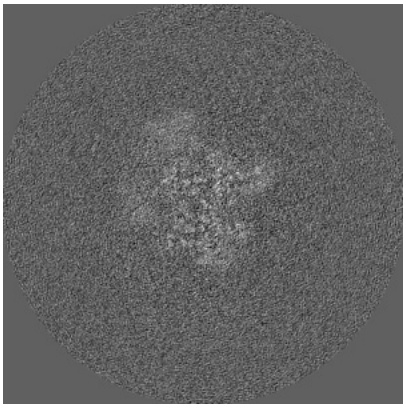

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

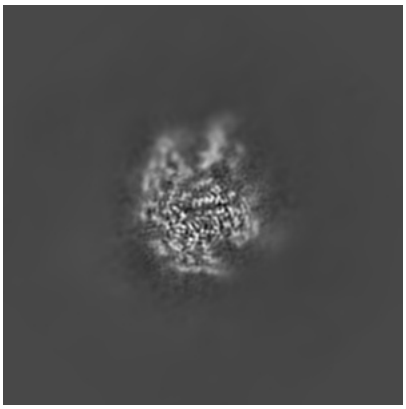

Y Index: 180

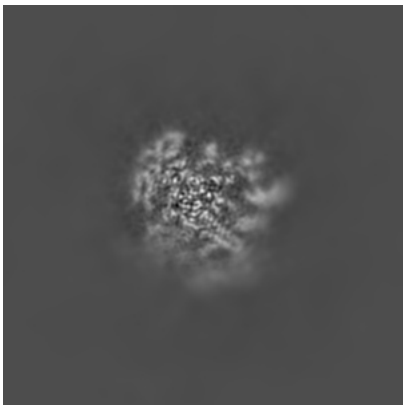

Z Index: 180

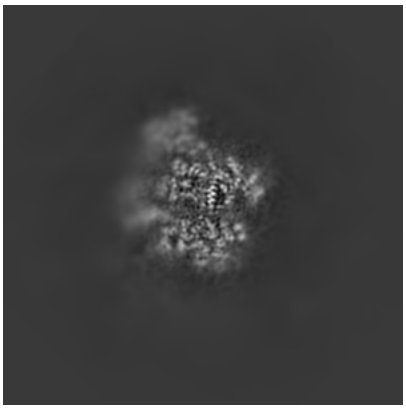
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

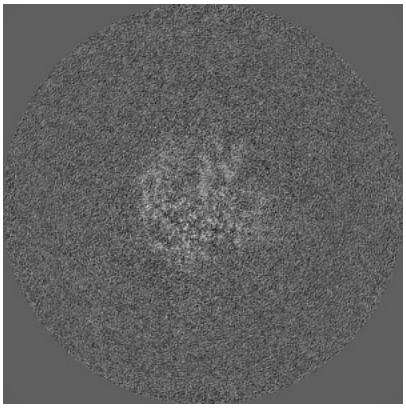
6.3.1 Primary map

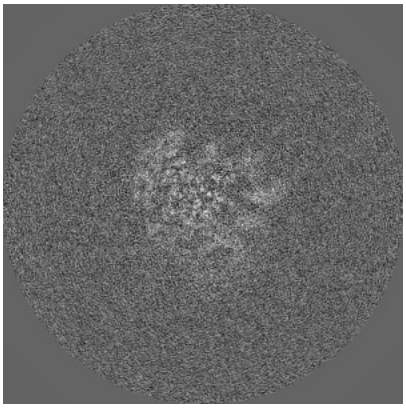

X Index: 186

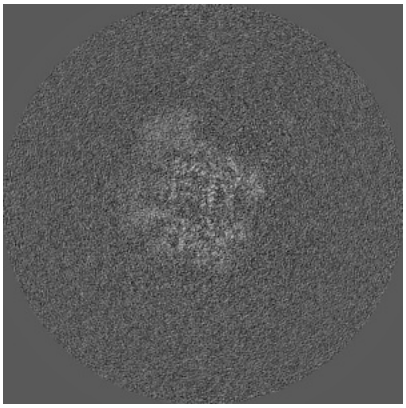

Y Index: 190


Z Index: 185

6.3.2 Raw map


X Index: 179

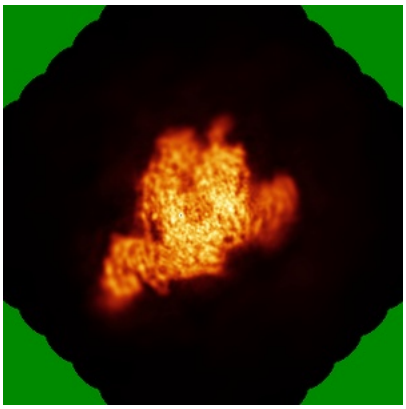

Y Index: 190


Z Index: 185

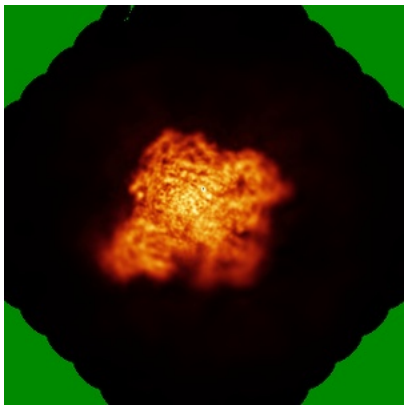
The images above show the largest variance slices of the map in three orthogonal directions.

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

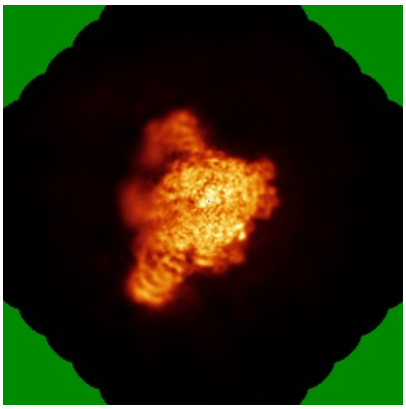
6.4.1 Primary map



X

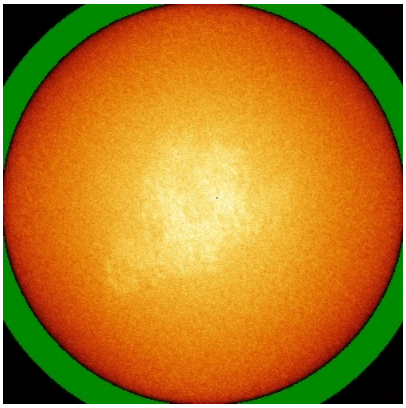


Y

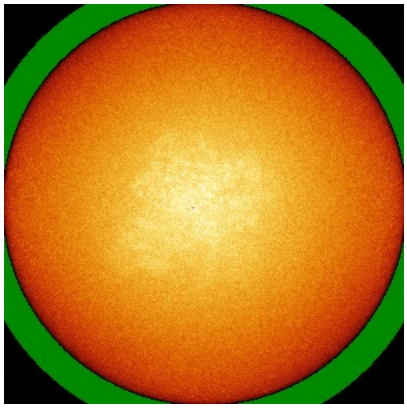


Z

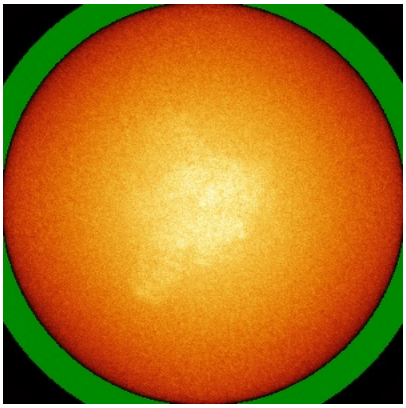
6.4.2 Raw map



X



Y

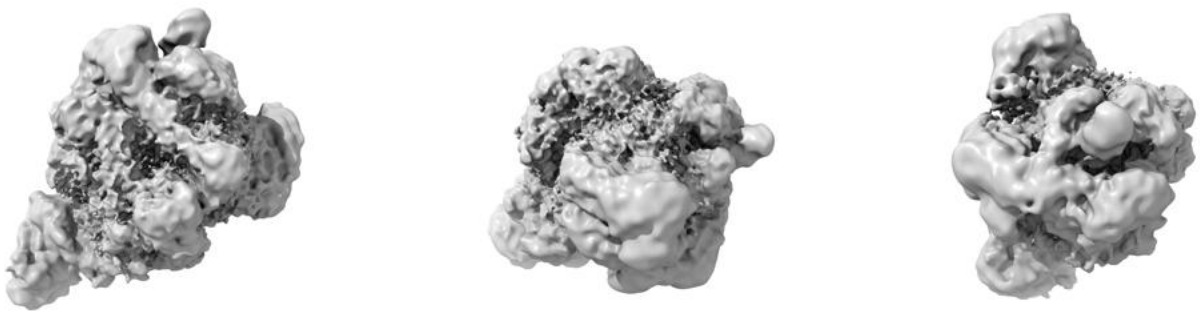


Z

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

6.5 Orthogonal surface views (i)

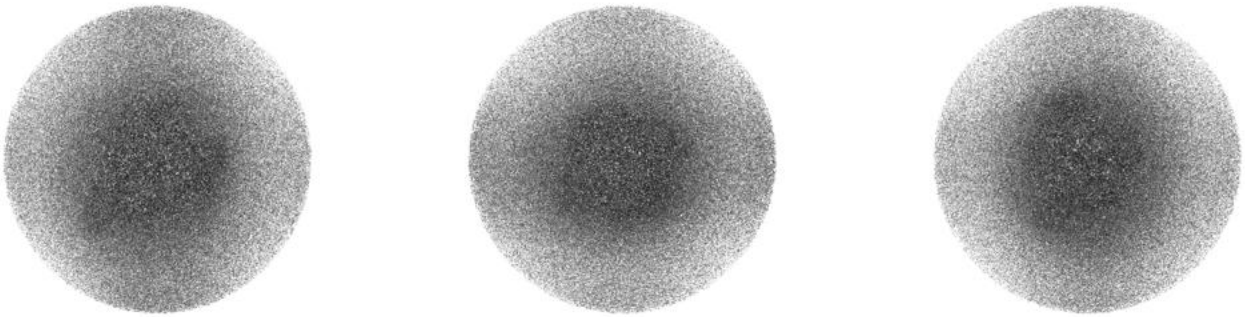
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

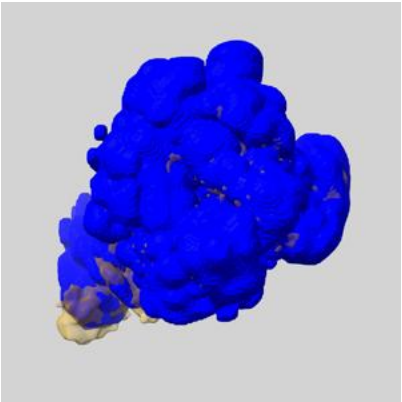
6.6 Mask visualisation (i)

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

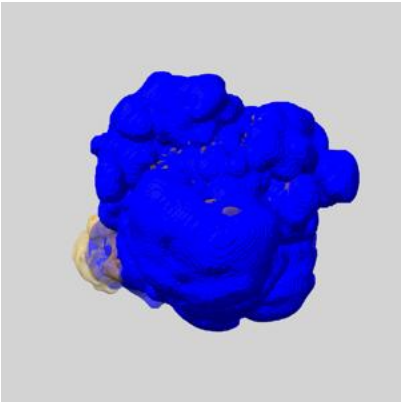
A mask typically either:

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

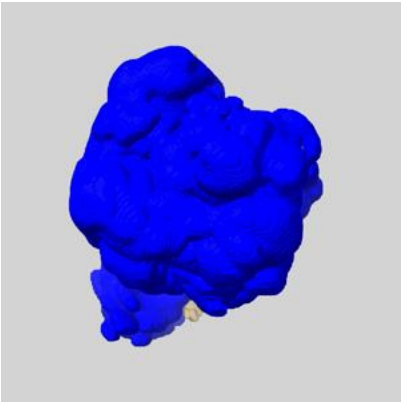
6.6.1 emd_19022_msk_1.map (i)



X



Y

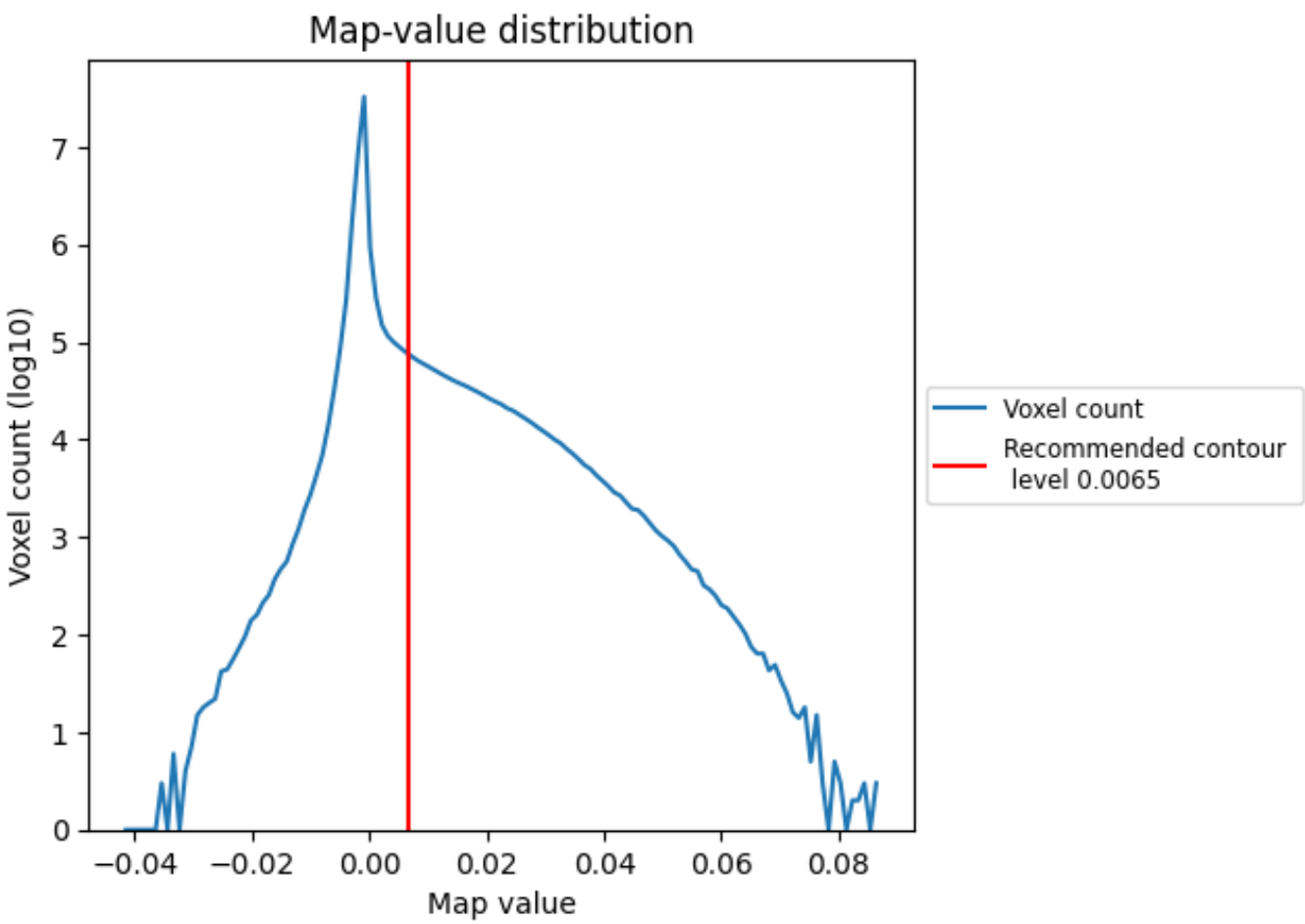


Z

7 Map analysis (i)

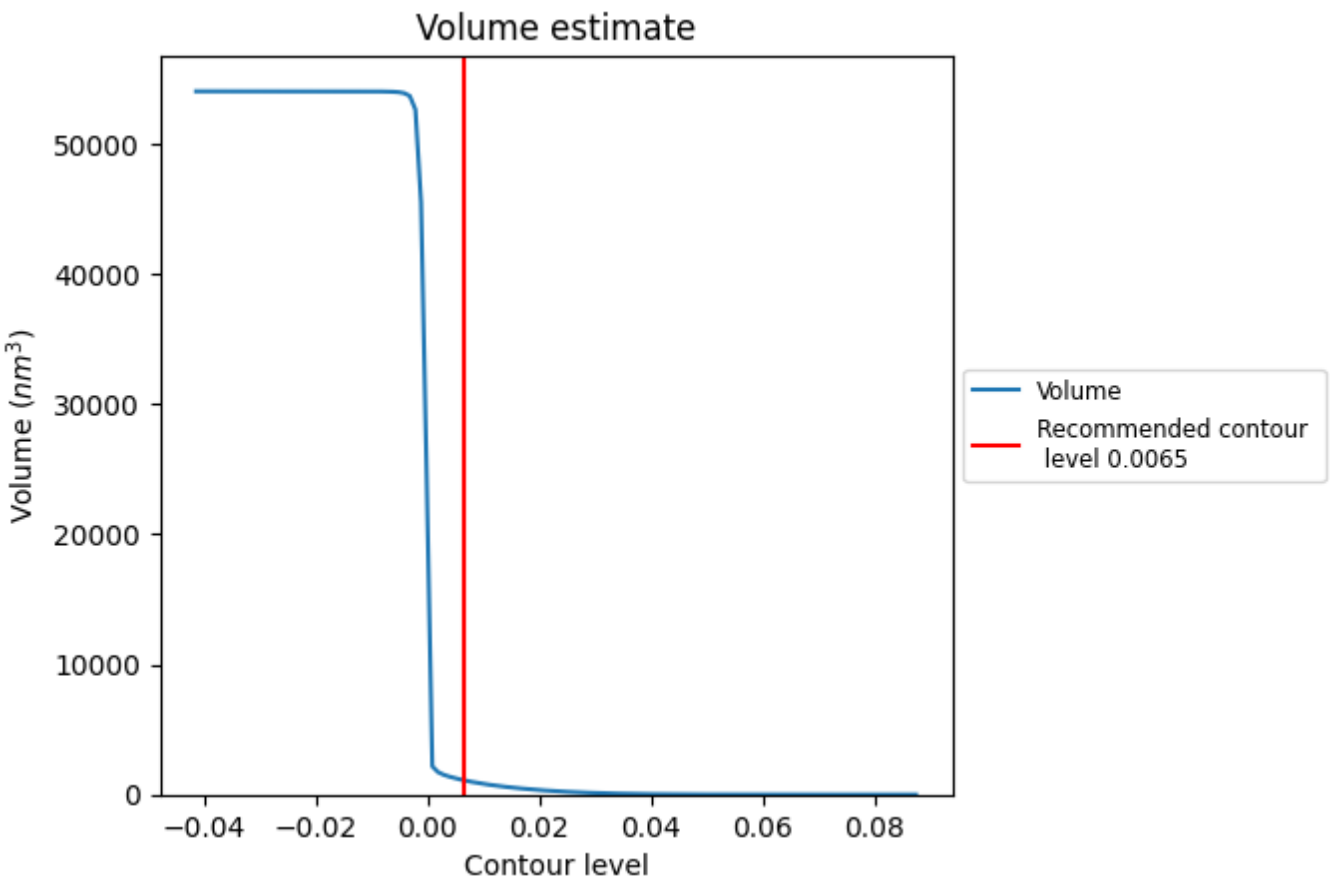
This section contains the results of statistical analysis of the map.

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.

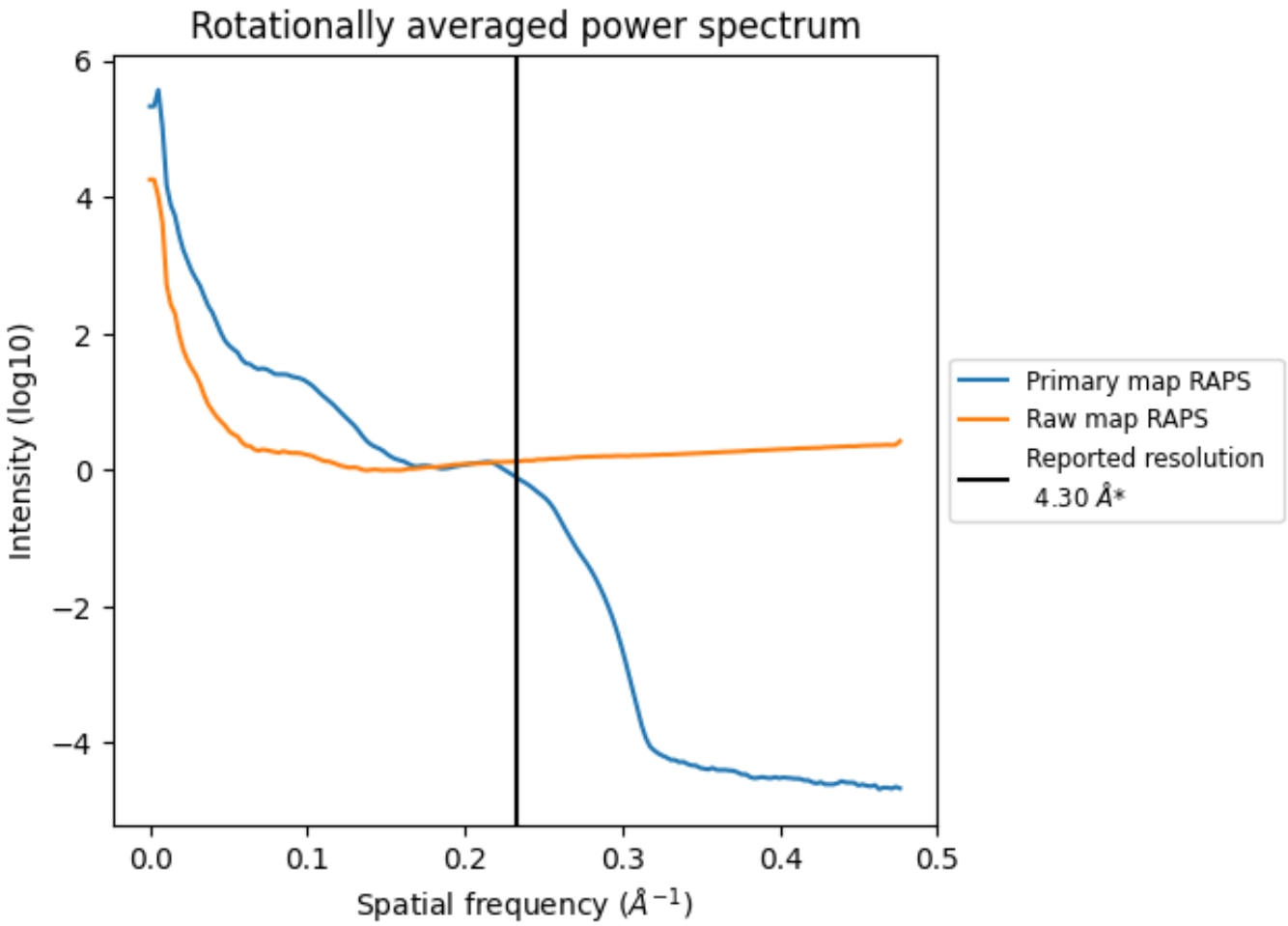
7.2 Volume estimate (i)



The volume at the recommended contour level is 1093 nm^3; this corresponds to an approximate mass of 987 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

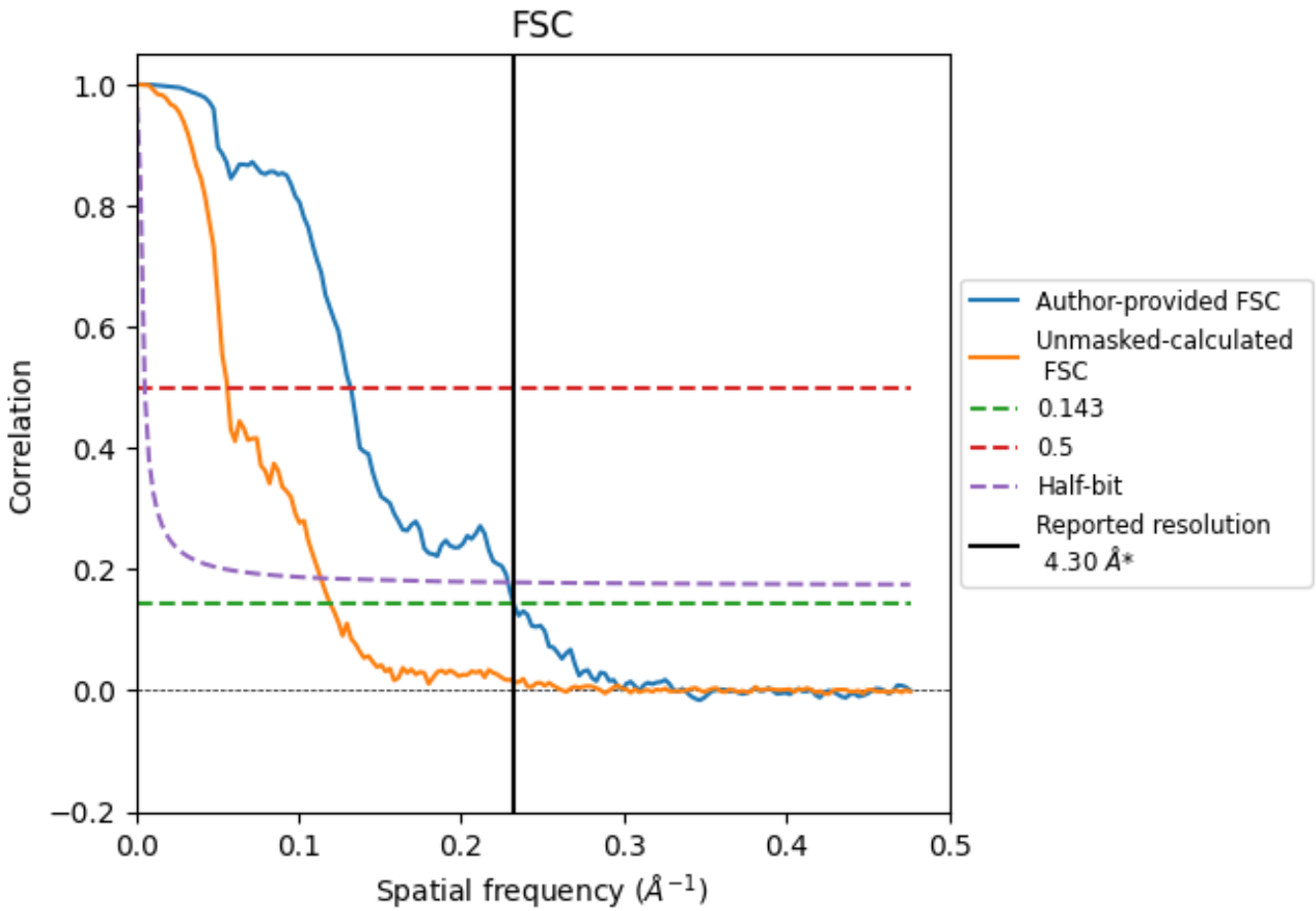


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (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 0.233 Å^{-1}

8.2 Resolution estimates (i)

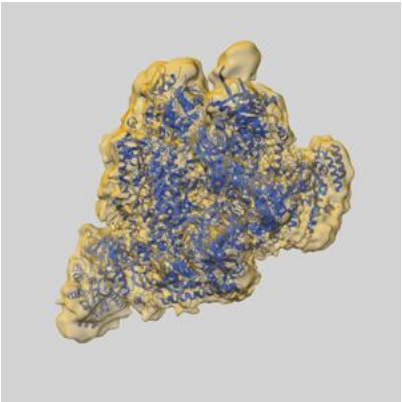
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.31	7.58	4.37
Unmasked-calculated*	8.38	17.89	8.80

*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 8.38 differs from the reported value 4.3 by more than 10 %

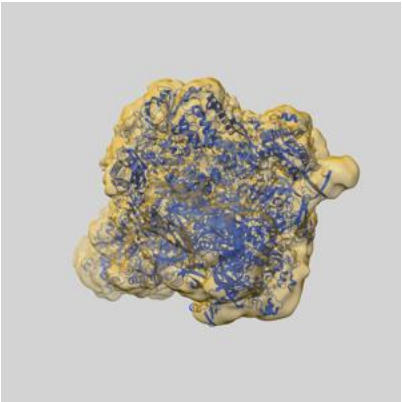
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19022 and PDB model 8RAP. Per-residue inclusion information can be found in section 3 on page 9.

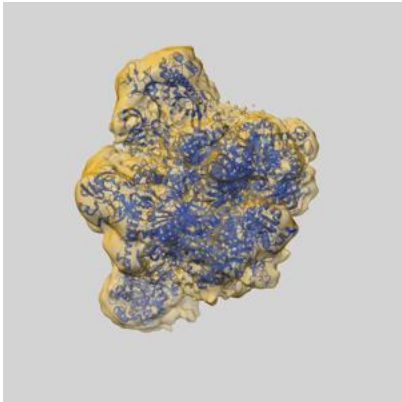
9.1 Map-model overlay (i)



X



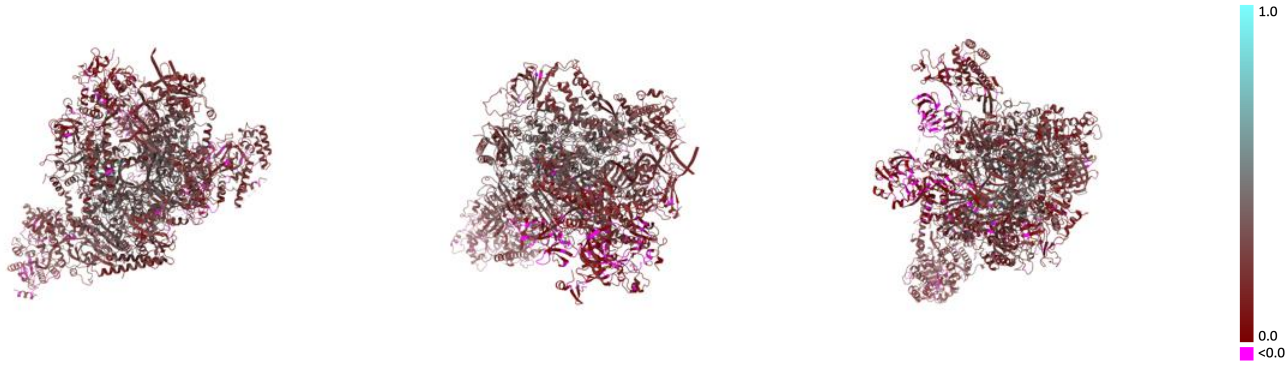
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

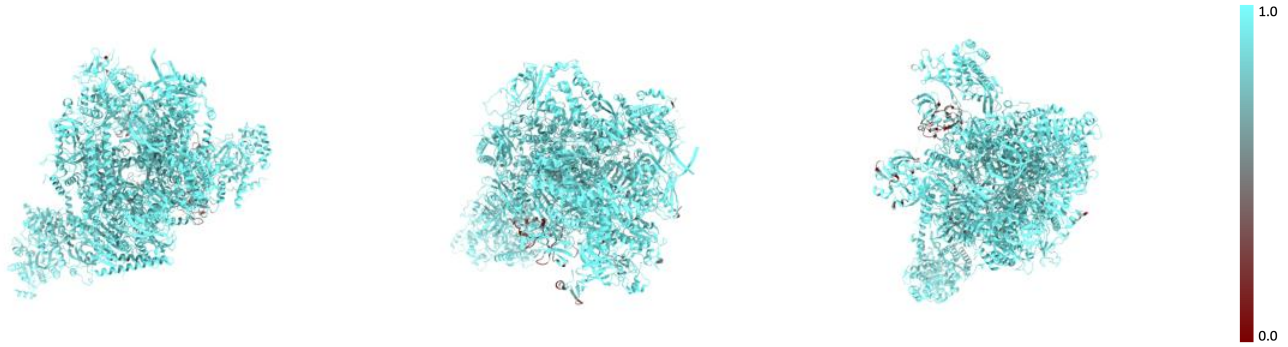
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

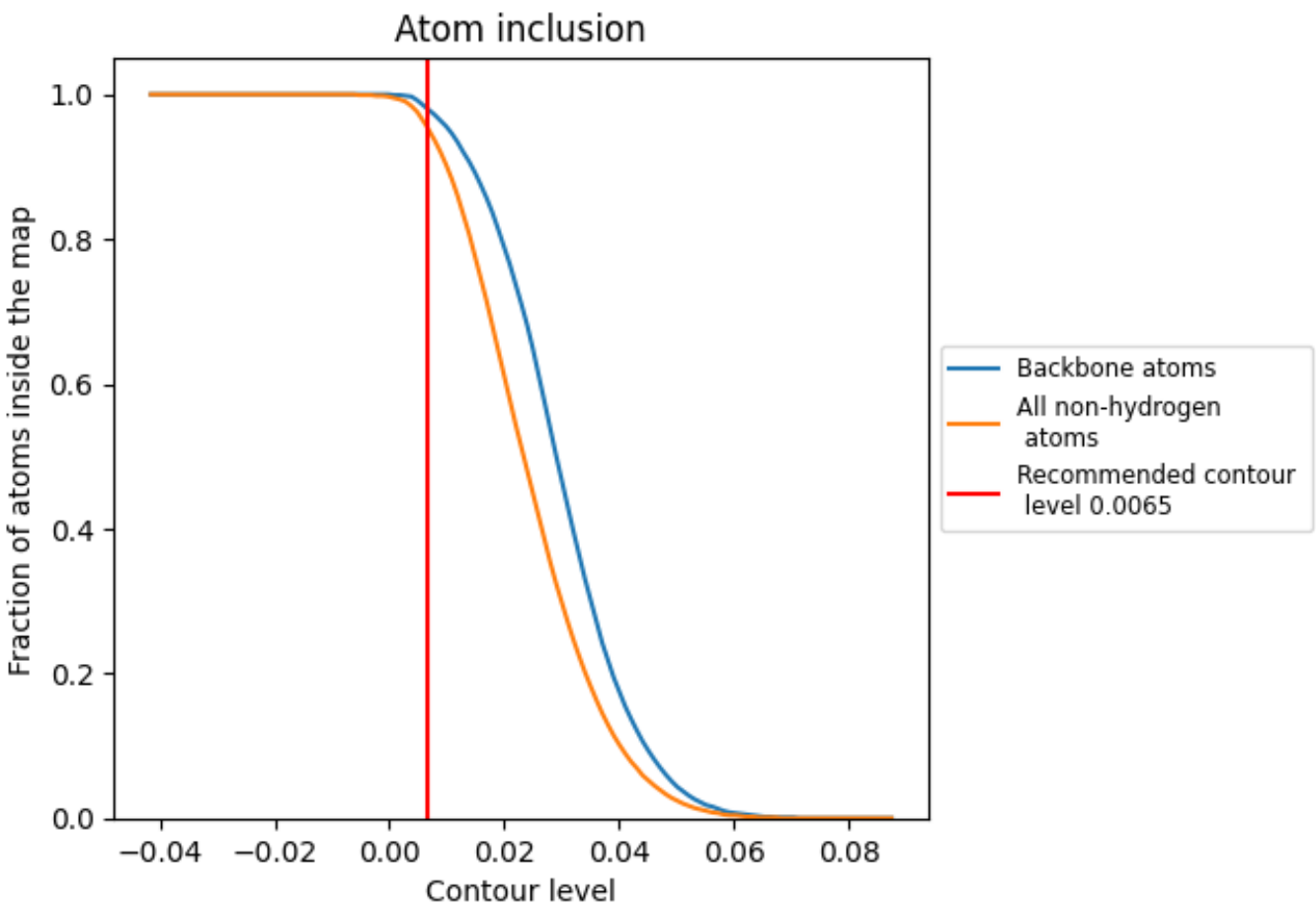
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0065).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.2400
A	0.9660	0.2910
B	0.9660	0.3020
C	0.9660	0.3130
D	0.9830	0.1600
E	0.9820	0.2750
F	0.9790	0.2940
G	0.9750	0.1620
H	0.9820	0.2430
I	0.9820	0.1500
J	0.9590	0.3350
K	0.9800	0.2720
L	0.9550	0.2900
M	0.8980	0.1210
N	0.9820	0.1840
O	0.9760	0.1680
P	0.9870	0.2190
T	0.9820	0.2400
Y	0.9290	0.0720
Z	0.7950	0.0850