wwPDB EM Validation Summary Report (i)

Mar 10, 2024 – 03:13 PM EDT

PDB ID	:	6PB5
EMDB ID	:	EMD-20287
Title	:	The E. coli class-II CAP-dependent transcription activation complex at the state 1 architecture
Authors	:	Liu, B.; Shi, W.
Deposited on	:	2019-06-13
Resolution	:	4.52 Å(reported)

This is a wwPDB EM Validation Summary 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 (1)) were used in the production of this report:

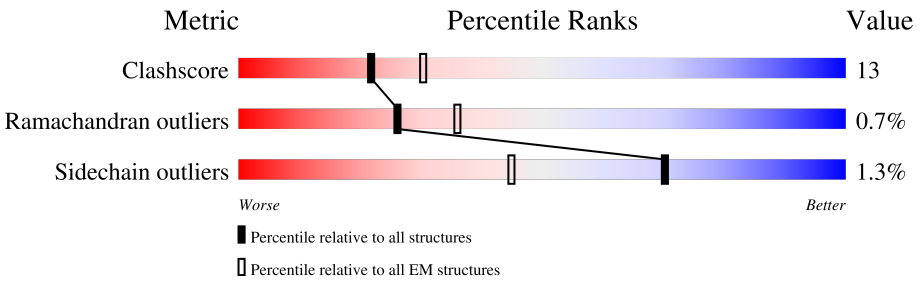
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.52 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	329	45% 21% • • 30%
1	B	329	40% 29% • 31%
2	C	1342	7% 64% 34% ••
3	D	1407	69% 25% • 5%
4	E	91	30% 67% 20% 13%
5	F	628	18% 60% 16% • 23%
6	G	210	60% 69% 24% • 6%
6	H	210	48% 77% 16% 6%

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Mol	Chain	Length	Quality of chain
7	1	78	24% 78% 15% 6%
8	2	78	28% 85% 15%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 69718 atoms, of which 34341 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 alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	230	3599	1112	1813	317	351	6	0	0
1	B	228	3556	1100	1789	312	349	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	1334	21054	6603	10532	1831	2045	43	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	1337	21012	6531	10616	1853	1962	50	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	79	1261	382	634	118	126	1	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	482	7892	2449	3975	700	745	23	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a protein called cAMP-activated global transcriptional regulator CRP.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	197	3154	986	1598	273	288	9	0	0
6	H	197	3155	986	1599	273	288	9	0	0

- Molecule 7 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	1	78	2480	765	889	264	484	78	0	0

- Molecule 8 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	2	78	2486	767	874	313	454	78	0	0

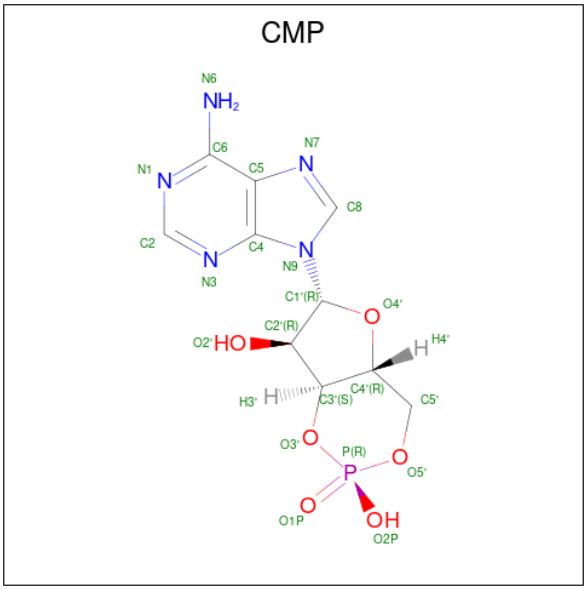
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	D	2	2	2	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	D	1	1	1	0

- Molecule 11 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



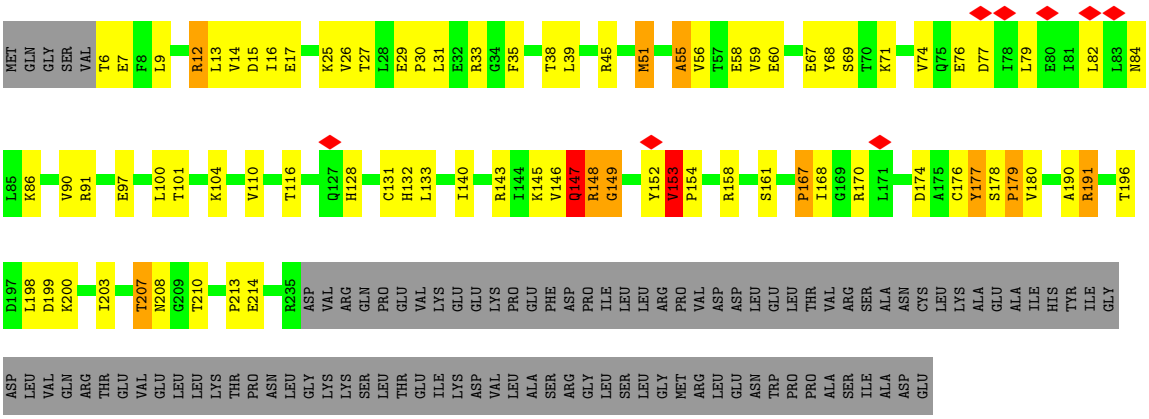
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
11	G	1	33	10	11	5	6	1	0
			Total	C	H	N	O	P	
11	H	1	33	10	11	5	6	1	0

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.

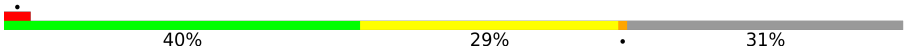
• Molecule 1: DNA-directed RNA polymerase subunit alpha

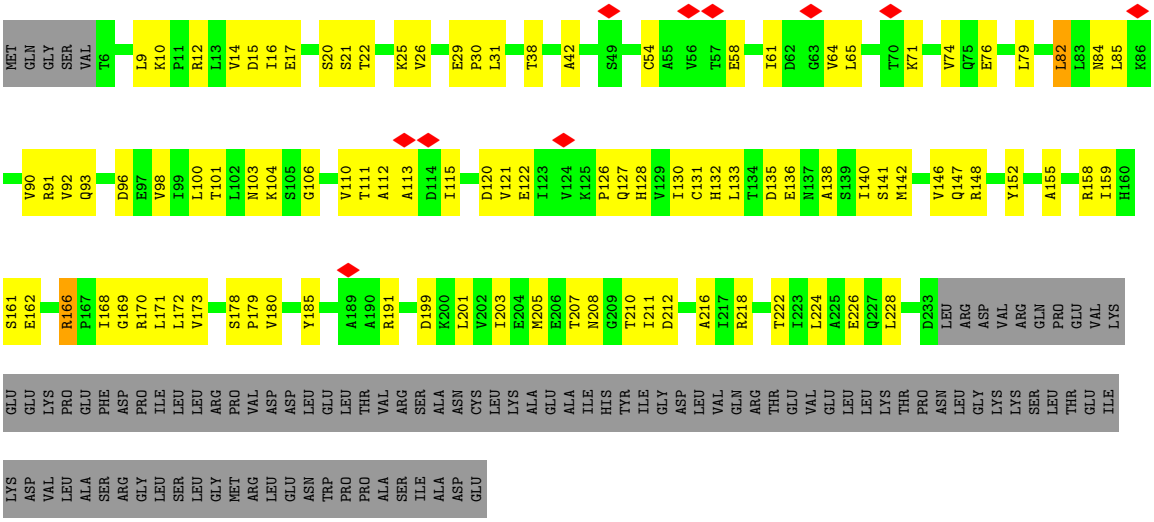
Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

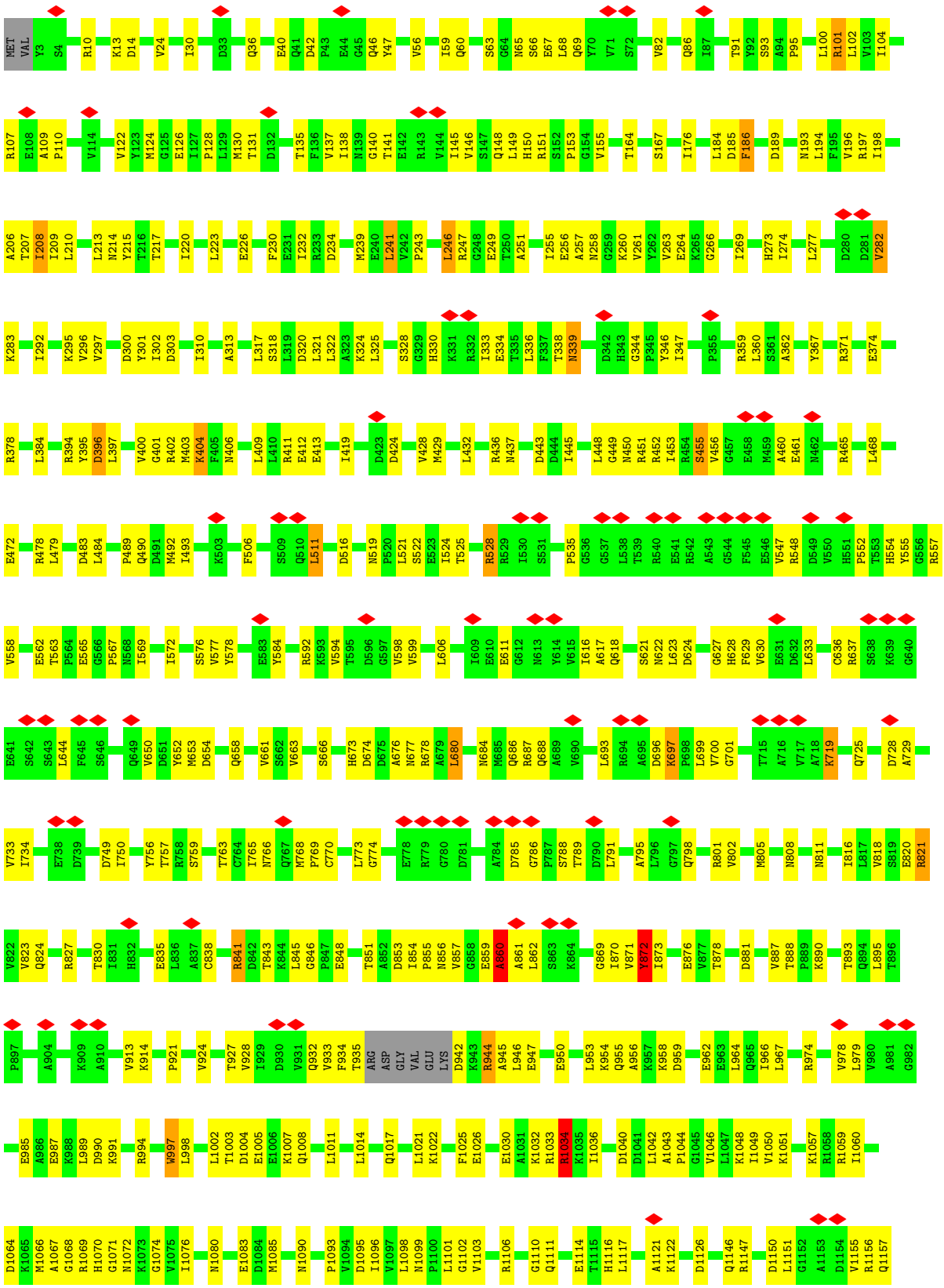


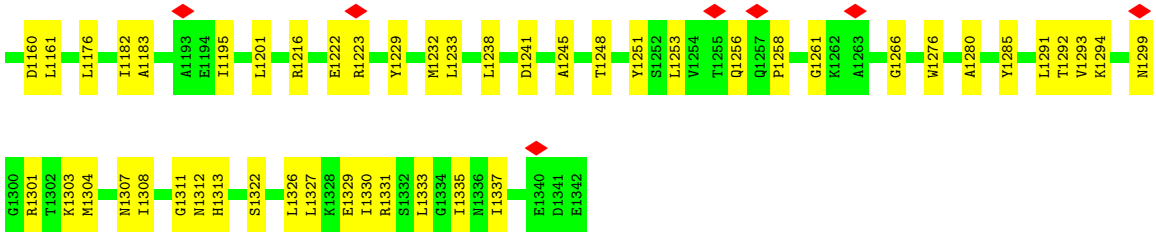


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

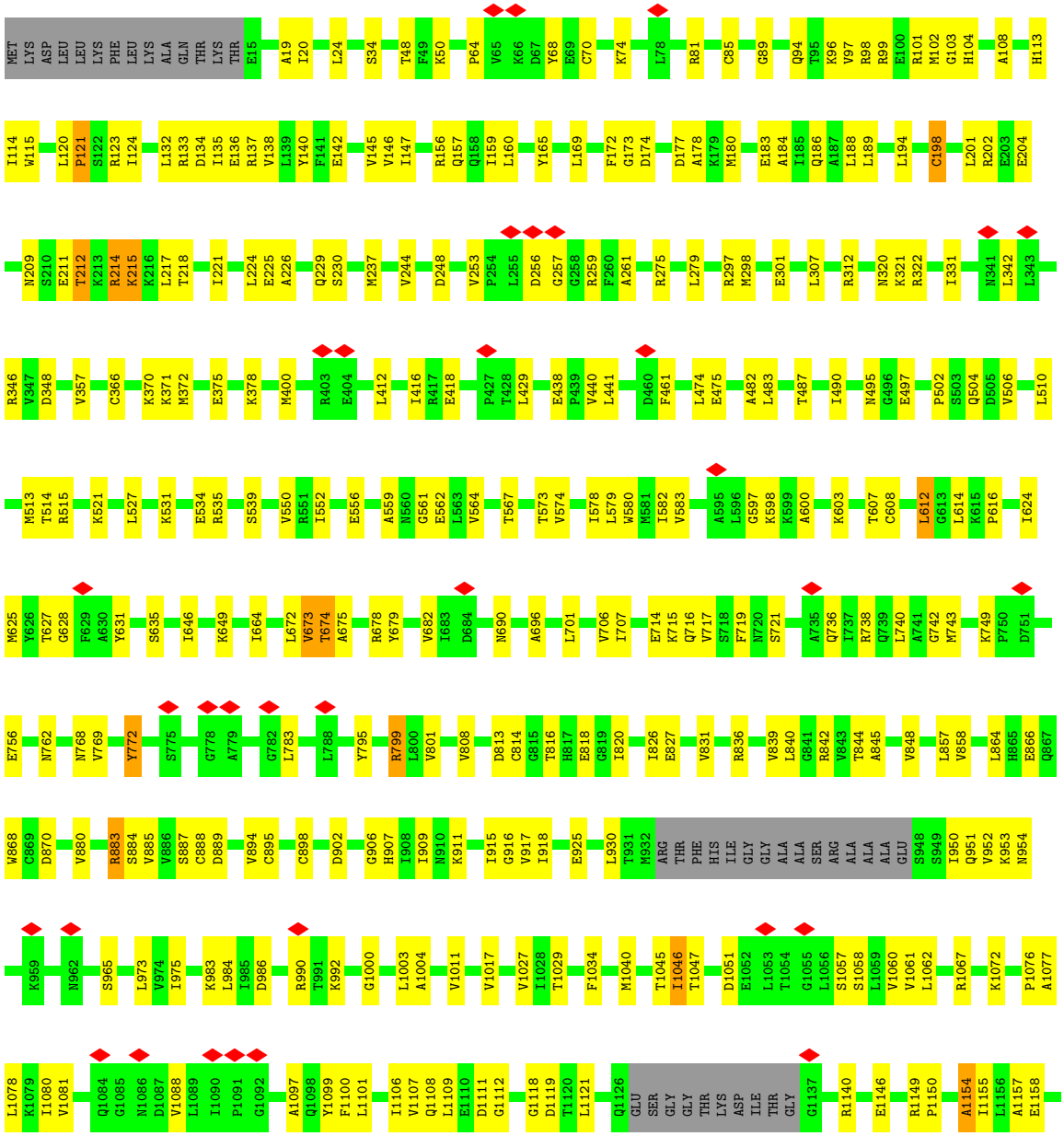
7%
64%
34%

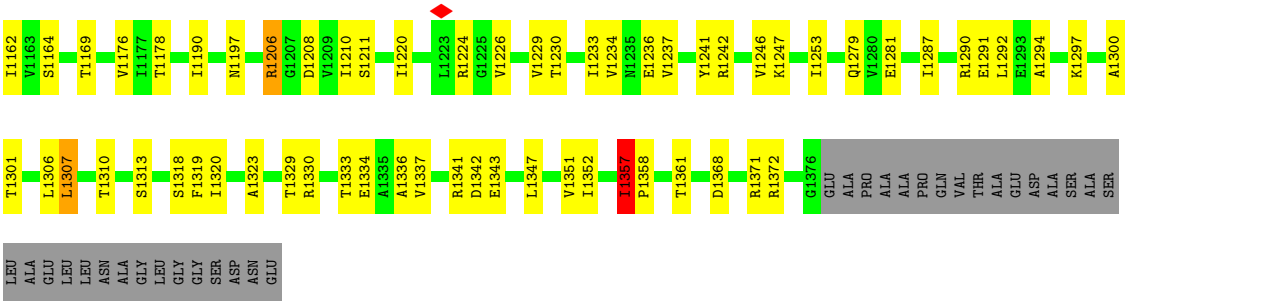

MET VAL Y3 S4 R10 K13 D14 V24 I30 D33 Q36 E40 Q41 D42 P43 E44 G45 Q46 Y47 V56 I59 Q60 S63 G64 N65 S66 E67 L68 Q69 Y70 V71 S72 V82 Q86 I87 T91 Y92 S93 A94 P95 L100 R101 L102 V103 I104
R107 E108 A109 P110 V114 V122 Y123 M124 G125 E126 I127 P128 L129 M130 T131 D132 T135 F136 V137 I138 N139 G140 T141 E142 R143 V144 I145 V146 S147 Q148 L149 H150 R151 S152 P153 G154 V155 T164 S167 I176 L184 D185 F186 D189 N193 L194 F195 V196 R197 I198
A206 T207 I208 I209 L210 L213 N214 Y215 T216 T217 I220 L223 E226 F230 E231 I232 R233 D234 M239 E240 L241 V242 P243 L246 R247 G248 E249 T250 A251 I255 E256 A257 N258 G259 K260 V261 Y262 V263 E264 K265 G266 I269 H273 I274 L277 D280 D281 V282
K283 I292 K295 V296 V297 D300 Y301 I302 D303 I310 A313 L317 S318 L319 D320 L321 L322 A323 K324 L325 S328 G329 H330 K331 R332 I333 E334 T335 L336 F337 T338 N339 D342 H343 G344 P345 Y346 I347 P355 R359 L360 S361 A362 Y367 R371 E374
R378 L384 R394 Y395 D396 L397 V400 G401 R402 M403 K404 F405 N406 L409 L410 R411 E412 E413 I419 D423 D424 V428 M429 L432 R436 N437 D443 D444 I445 L448 G449 N450 R451 R452 I453 R454 S455 V456 G457 E458 M459 A460 E461 N462 R465 L468
E472 R478 L479 D483 L484 P489 Q490 D491 M492 I493 K503 F506 S509 Q510 L511 D516 N519 P520 L521 S522 E523 I524 T525 R528 R529 T530 S531 P535 G536 G537 L538 T539 R540 E541 R542 A543 G544 F545 E546 V547 R548 D549 V550 H551 P552 T553 H554 Y555 G556 R557
V558 E562 T563 P564 E565 G566 P567 N568 I569 I572 S576 V577 Y578 E583 Y584 R592 K593 V594 T595 D596 G597 V598 V599 L606 I609 E610 E611 G612 N613 Y614 V615 I616 A617 Q618 S621 N622 L623 D624 G627 H628 F629 V630 E631 D632 L633 C636 R637 S638 K639 G640
E641 S642 S643 L644 F645 S646 Q649 V650 D651 Y652 M653 D654 Q658 V661 S662 V663 S666 H673 D674 D675 A676 N677 R678 A679 L680 N684 M685 Q686 R687 Q688 A689 V690 L693 R694 A695 D696 K697 P698 L699 V700 G701 T715 A716 V717 A718 K719 Q725 D728 A729
V733 I734 E738 D739 D749 I750 Y756 T757 R758 S759 T763 C764 I765 N766 Q767 M768 P769 C770 L773 G774 E778 R779 G780 D781 A784 D785 G786 P787 S788 T789 D790 L791 A795 L796 G797 Q798 R801 V802 M805 N808 N811 I816 L817 V818 S819 E820 R821
V822 V823 Q824 R827 T830 I831 H832 E835 L836 A837 C838 R841 D842 T843 K844 L845 G846 P847 E848 T851 A852 D853 I854 P855 N856 V857 G858 E859 A860 A861 L862 S863 K864 G869 I870 V871 Y872 I873 E876 V877 T878 D881 V887 T888 P889 K890 T893 Q894 L895 T896
P897 A904 K909 A910 V913 K914 P921 V924 T927 V928 I929 D930 V931 Q932 V933 F934 T935 ARG ASP GLY VAL GLU LYS D942 K943 R944 A945 L946 E947 E950 L953 K954 Q955 A956 K957 K958 D959 E962 E963 L964 Q965 I966 L967 R974 V978 L979 V980 A981 G982
E985 A986 E987 K988 L989 D990 K991 R994 W997 L998 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 L1011 L1014 Q1017 L1021 K1022 F1025 E1026 E1030 A1031 K1032 R1033 R1034 K1035 I1036 D1040 D1041 L1042 A1043 P1044 G1045 V1046 L1047 K1048 I1049 V1050 K1051 K1057 R1058 R1059 I1060
D1064 K1065 M1066 A1067 G1068 R1069 H1070 G1071 N1072 K1073 G1074 V1075 I1076 N1080 E1083 D1084 M1085 N1090 P1093 V1094 D1095 I1096 V1097 L1098 N1099 P1100 L1101 G1102 V1103 R1106 G1110 Q1111 E1114 T1115 H1116 L1117 A1121 K1122 D1126 Q1146 R1147 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157



• Molecule 3: DNA-directed RNA polymerase subunit beta'

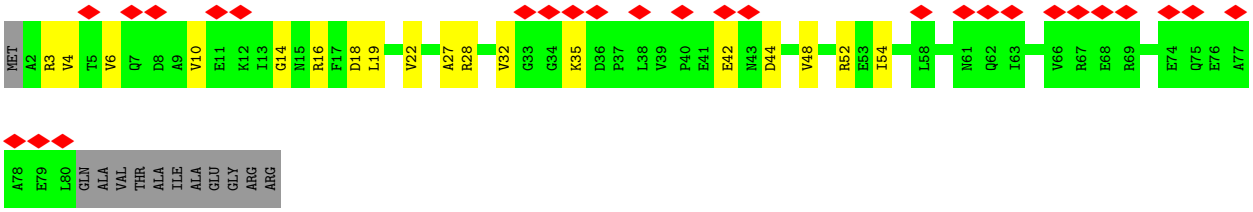
Chain D:





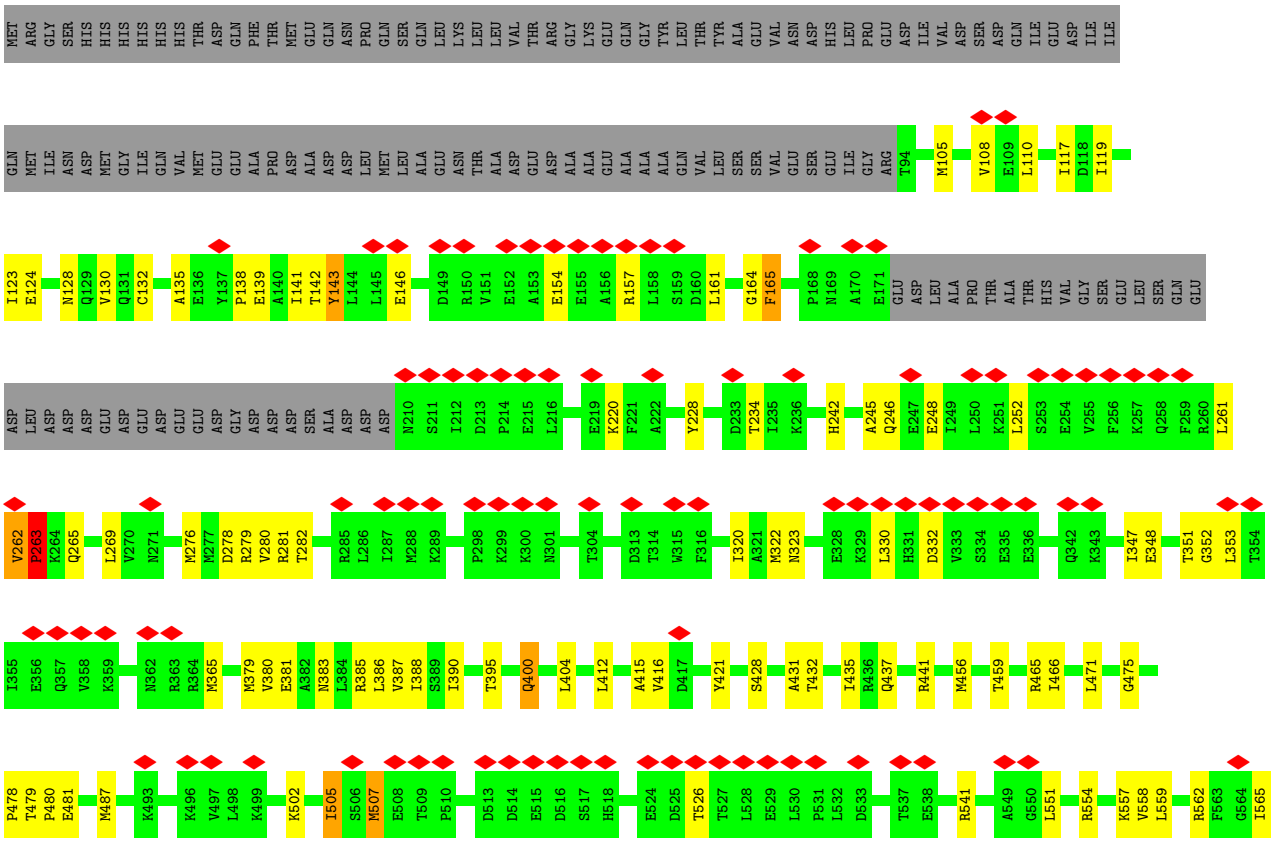
• Molecule 4: DNA-directed RNA polymerase subunit omega

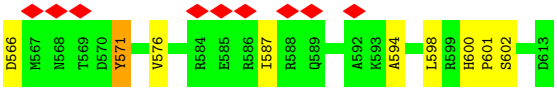
Chain E:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



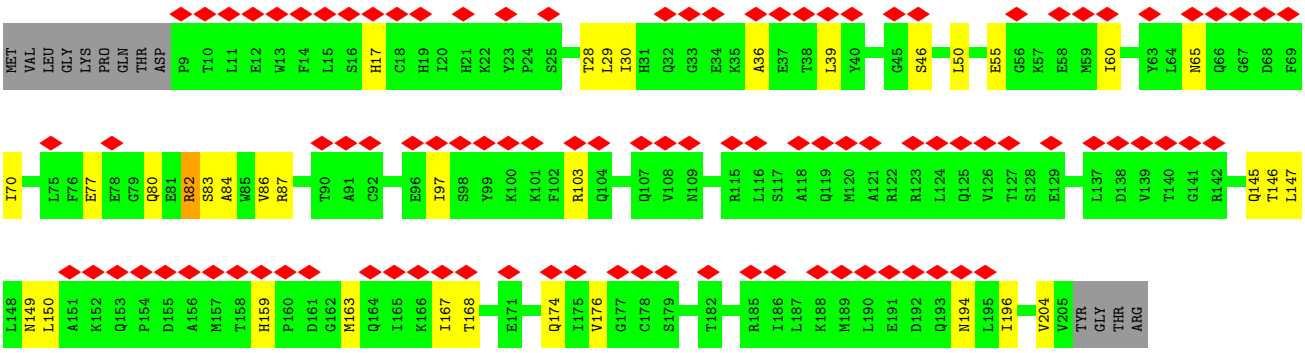


• Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain G:

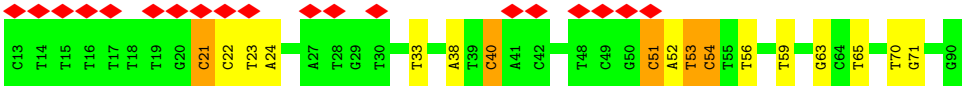
• Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain H:



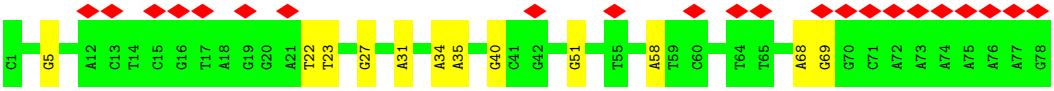
• Molecule 7: SYNTHETIC NONTEMPLATE STRAND DNA (78-MER)

Chain 1:



• Molecule 8: SYNTHETIC TEMPLATE STRAND DNA (78-MER)

Chain 2:


C1
G5
A12
C13
T14
C15
G16
T17
A18
G19
G20
A21
T22
T23
G27
A31
A34
A35
G40
C41
G42
G51
T55
A58
T59
C60
T64
T65
A68
G69
G70
C71
A72
A73
A74
A75
A76
A77
G78

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.780	Depositor
Minimum map value	-1.761	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	0.262	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	345.59998, 345.59998, 345.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8999999, 0.8999999, 0.8999999	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: MG, CMP, 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	0.55	0/1808	0.87	3/2450 (0.1%)
1	B	0.55	0/1789	0.79	2/2425 (0.1%)
2	C	0.54	1/10690 (0.0%)	0.79	11/14423 (0.1%)
3	D	0.50	4/10553 (0.0%)	0.76	4/14248 (0.0%)
4	E	0.37	0/629	0.62	0/847
5	F	0.46	1/3971 (0.0%)	0.73	2/5340 (0.0%)
6	G	0.47	0/1580	0.77	2/2127 (0.1%)
6	H	0.49	0/1580	0.77	1/2127 (0.0%)
7	1	1.11	3/1777 (0.2%)	1.27	8/2741 (0.3%)
8	2	1.02	2/1815 (0.1%)	1.08	1/2800 (0.0%)
All	All	0.59	11/36192 (0.0%)	0.83	34/49528 (0.1%)

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	10
1	B	0	1
2	C	0	20
3	D	0	11
5	F	0	9
6	H	0	3
All	All	0	54

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	772	TYR	CD2-CE2	-7.59	1.27	1.39
8	2	35	DA	C3'-O3'	6.44	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	51	DC	C1'-N1	5.88	1.56	1.49
7	1	21	DC	C1'-N1	5.57	1.56	1.49
8	2	31	DA	N9-C4	-5.52	1.34	1.37

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	82	ARG	NE-CZ-NH2	-9.29	115.65	120.30
2	C	821	ARG	NE-CZ-NH2	-8.77	115.92	120.30
2	C	528	ARG	NE-CZ-NH1	8.54	124.57	120.30
3	D	1206	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	C	680	LEU	CA-CB-CG	7.81	133.26	115.30

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLY	Peptide
1	A	51	MET	Peptide
1	A	55	ALA	Peptide
1	A	68	TYR	Peptide
1	A	77	ASP	Peptide

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	1786	1813	1813	65	0
1	B	1767	1789	1789	81	0
2	C	10522	10532	10533	358	0
3	D	10396	10616	10616	273	0
4	E	627	634	634	19	0
5	F	3917	3975	3977	75	0
6	G	1556	1598	1600	51	0
6	H	1556	1599	1600	24	0
7	1	1591	889	891	17	0
8	2	1612	874	876	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	G	22	11	11	2	0
11	H	22	11	11	5	0
All	All	35377	34341	34351	884	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 13.

The worst 5 of 884 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)
11:H:301:CMP:H2	11:H:301:CMP:C2	0.97	1.50
11:G:301:CMP:H2	11:G:301:CMP:C2	0.97	1.48
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.44	0.90
1:A:16:ILE:HD11	1:A:214:GLU:HB2	1.58	0.84
2:C:563:THR:OG1	2:C:572:ILE:O	1.97	0.83

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	228/329 (69%)	192 (84%)	30 (13%)	6 (3%)	5 34
1	B	226/329 (69%)	205 (91%)	21 (9%)	0	100 100
2	C	1330/1342 (99%)	1158 (87%)	161 (12%)	11 (1%)	19 60
3	D	1331/1407 (95%)	1155 (87%)	170 (13%)	6 (0%)	29 68
4	E	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	478/628 (76%)	418 (87%)	56 (12%)	4 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	195/210 (93%)	181 (93%)	14 (7%)	0	100	100
6	H	195/210 (93%)	178 (91%)	16 (8%)	1 (0%)	29	68
All	All	4060/4546 (89%)	3561 (88%)	471 (12%)	28 (1%)	26	62

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	C	339	ASN
2	C	860	ALA
2	C	861	ALA
2	C	872	TYR

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	198/286 (69%)	195 (98%)	3 (2%)	65	80
1	B	196/286 (68%)	196 (100%)	0	100	100
2	C	1150/1157 (99%)	1134 (99%)	16 (1%)	67	81
3	D	1120/1168 (96%)	1106 (99%)	14 (1%)	69	82
4	E	67/75 (89%)	66 (98%)	1 (2%)	65	80
5	F	428/554 (77%)	421 (98%)	7 (2%)	62	79
6	G	170/181 (94%)	167 (98%)	3 (2%)	59	77
6	H	170/181 (94%)	169 (99%)	1 (1%)	86	92
All	All	3499/3888 (90%)	3454 (99%)	45 (1%)	70	82

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1149	ARG
5	F	220	LYS

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Mol	Chain	Res	Type
3	D	1206	ARG
3	D	1372	ARG
5	F	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1307	ASN
6	H	194	ASN
3	D	489	ASN
6	H	65	ASN
2	C	1314	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
11	CMP	G	301	-	22,25,25	1.49	4 (18%)	24,39,39	1.51	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CMP	H	301	-	22,25,25	1.59	5 (22%)	24,39,39	1.79	7 (29%)

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
11	CMP	G	301	-	-	0/0/31/31	0/4/4/4
11	CMP	H	301	-	-	0/0/31/31	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	301	CMP	P-O3'	3.77	1.64	1.57
11	G	301	CMP	P-O3'	3.57	1.63	1.57
11	H	301	CMP	P-O5'	3.52	1.61	1.57
11	G	301	CMP	P-O5'	3.11	1.61	1.57
11	H	301	CMP	O5'-C5'	-2.71	1.42	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	301	CMP	N3-C2-N1	-3.83	122.69	128.68
11	H	301	CMP	O3'-C3'-C2'	3.67	119.20	115.61
11	G	301	CMP	N3-C2-N1	-3.23	123.62	128.68
11	H	301	CMP	O2P-P-O3'	2.83	113.63	107.04
11	G	301	CMP	O5'-P-O3'	2.68	109.37	105.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

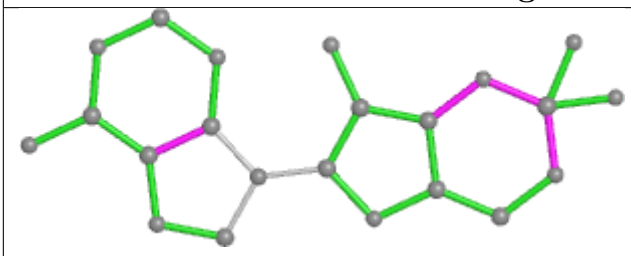
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	301	CMP	2	0
11	H	301	CMP	5	0

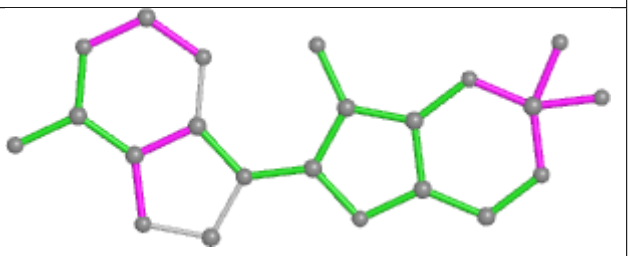
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

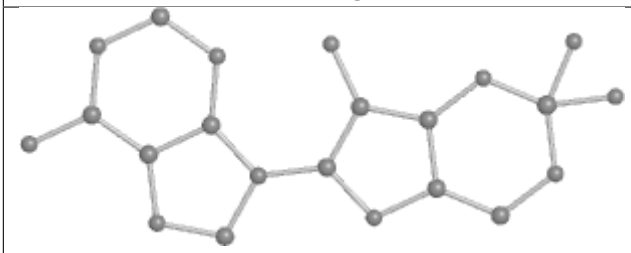
Ligand CMP G 301



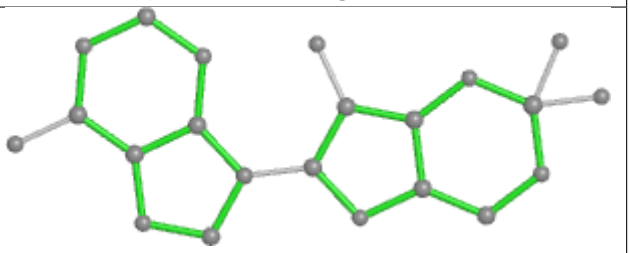
Bond lengths



Bond angles

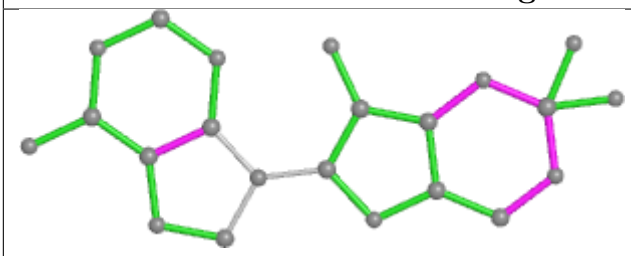


Torsions

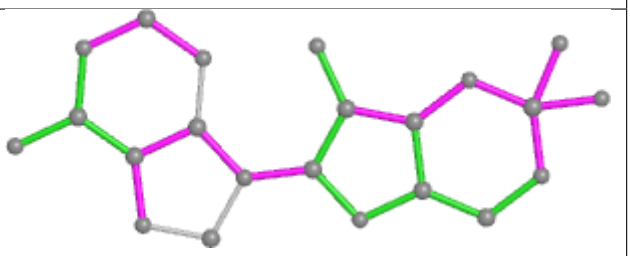


Rings

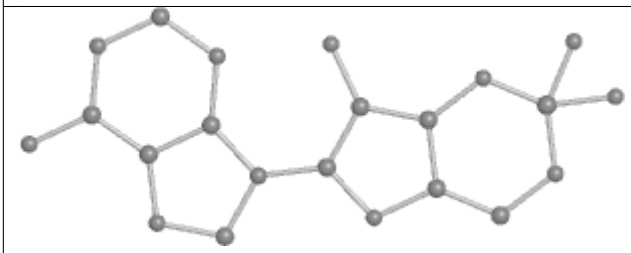
Ligand CMP H 301



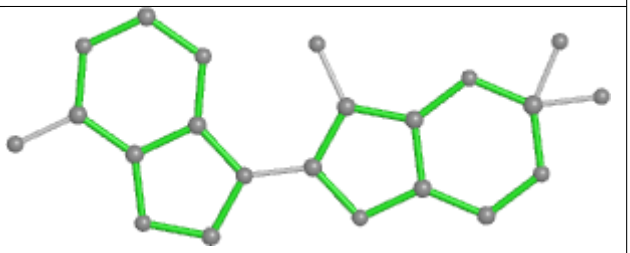
Bond lengths



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.

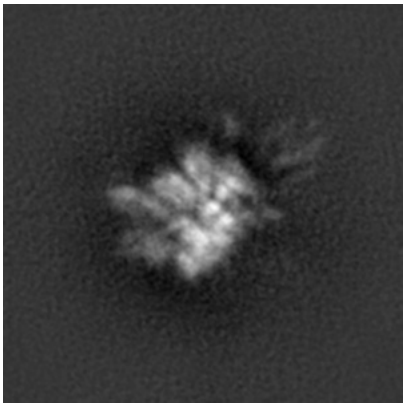
6 Map visualisation (i)

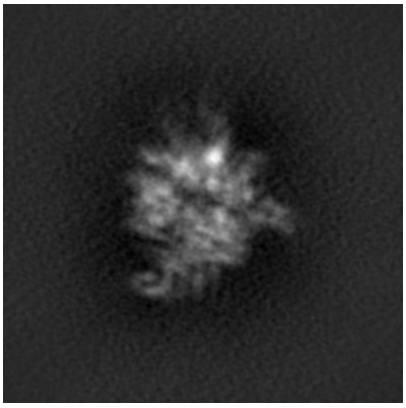
This section contains visualisations of the EMDB entry EMD-20287. These allow visual inspection of the internal detail of the map and identification of artifacts.

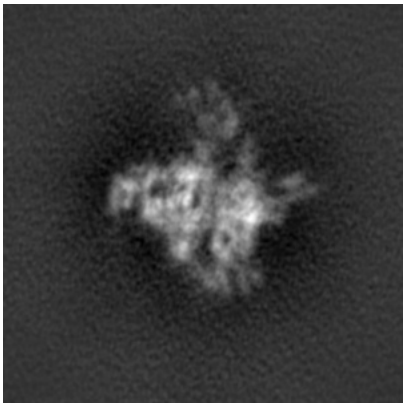
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

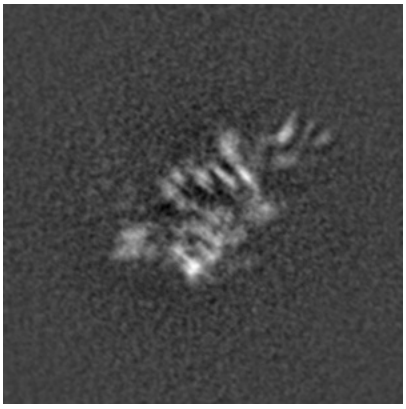

Y

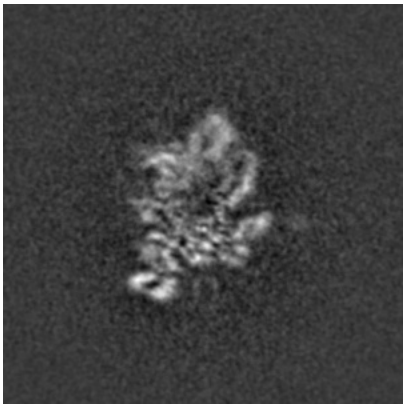

Z

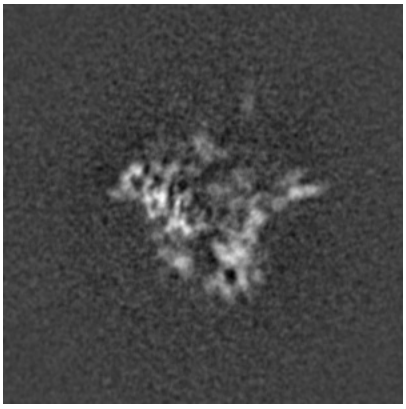
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 192

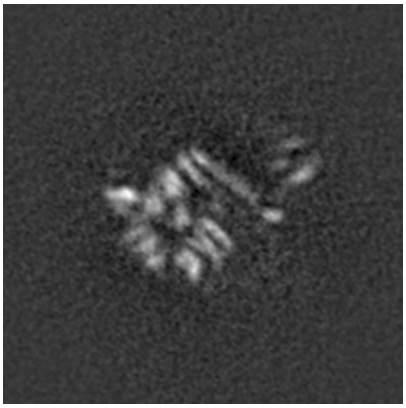

Y Index: 192


Z Index: 192

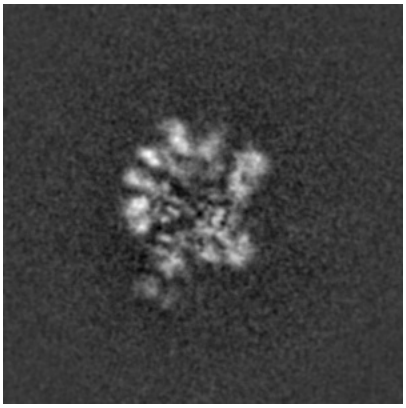
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

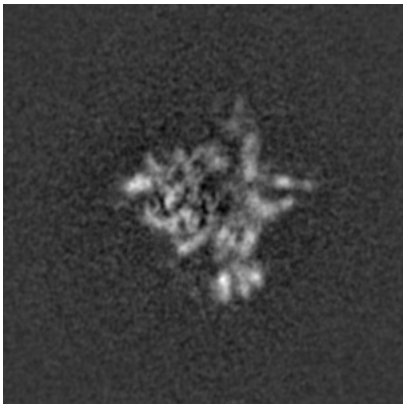
6.3.1 Primary map



X Index: 211



Y Index: 180

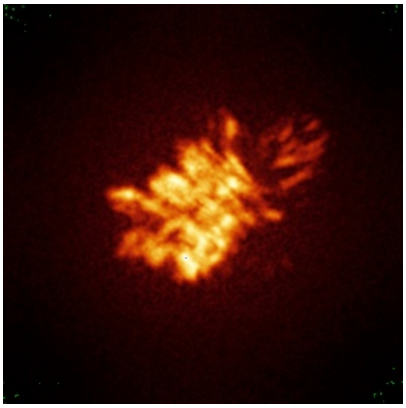


Z Index: 203

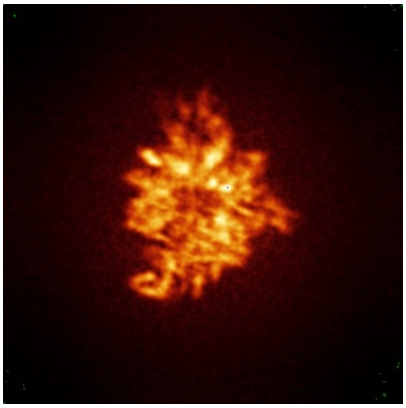
The images above show the largest variance slices of the map in three orthogonal directions.

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

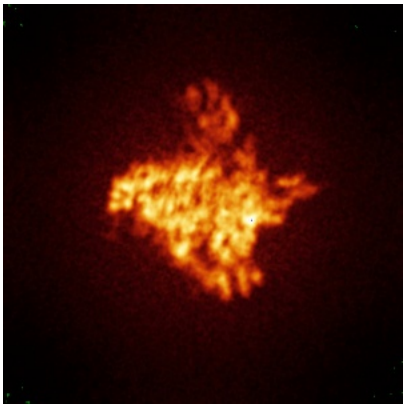
6.4.1 Primary map



X



Y

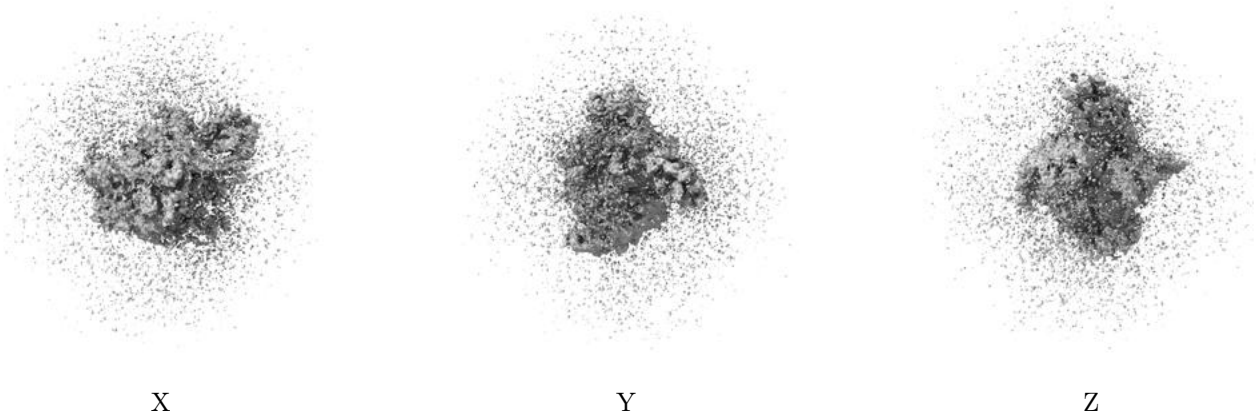


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

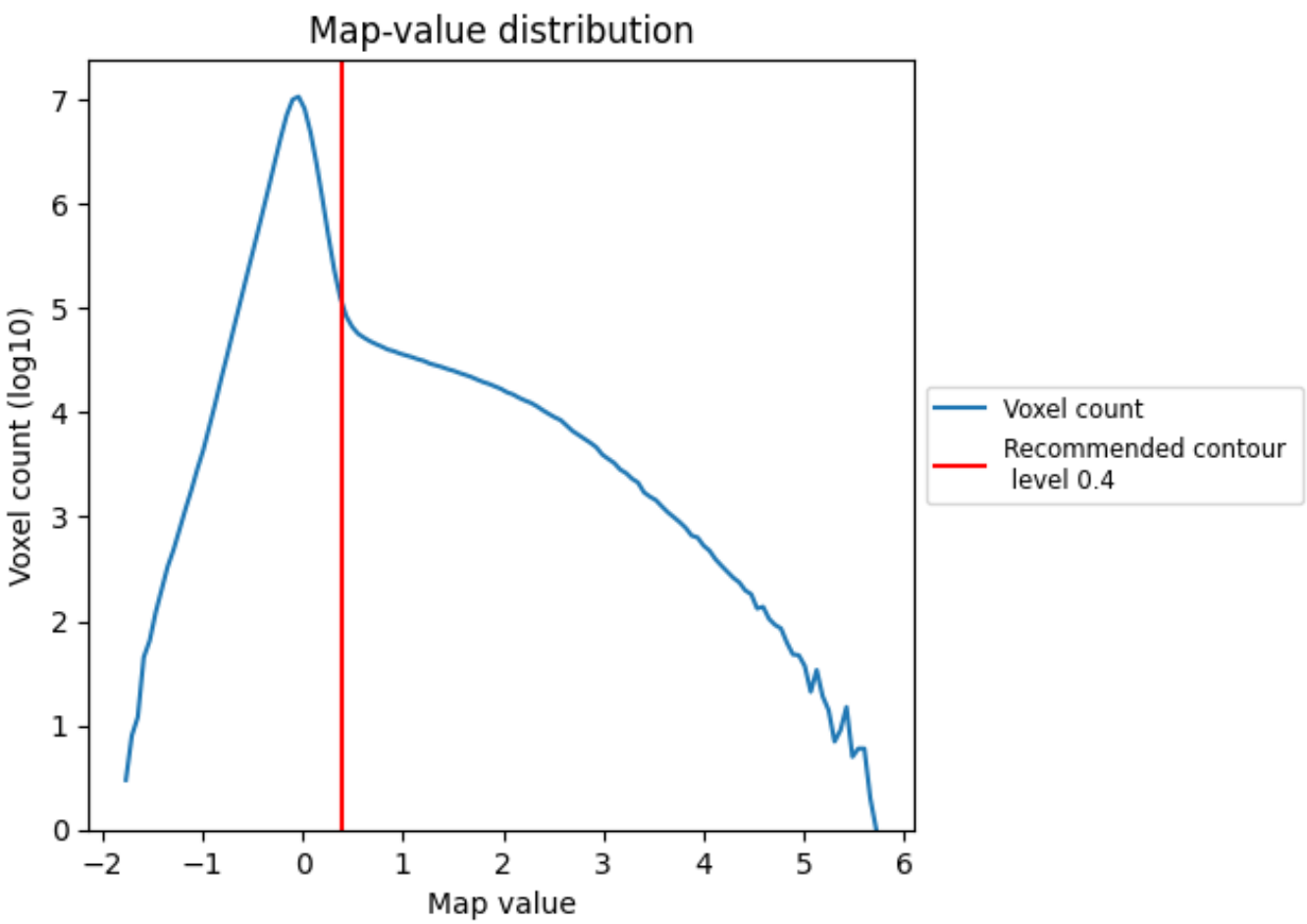
6.6 Mask visualisation (i)

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

7 Map analysis (i)

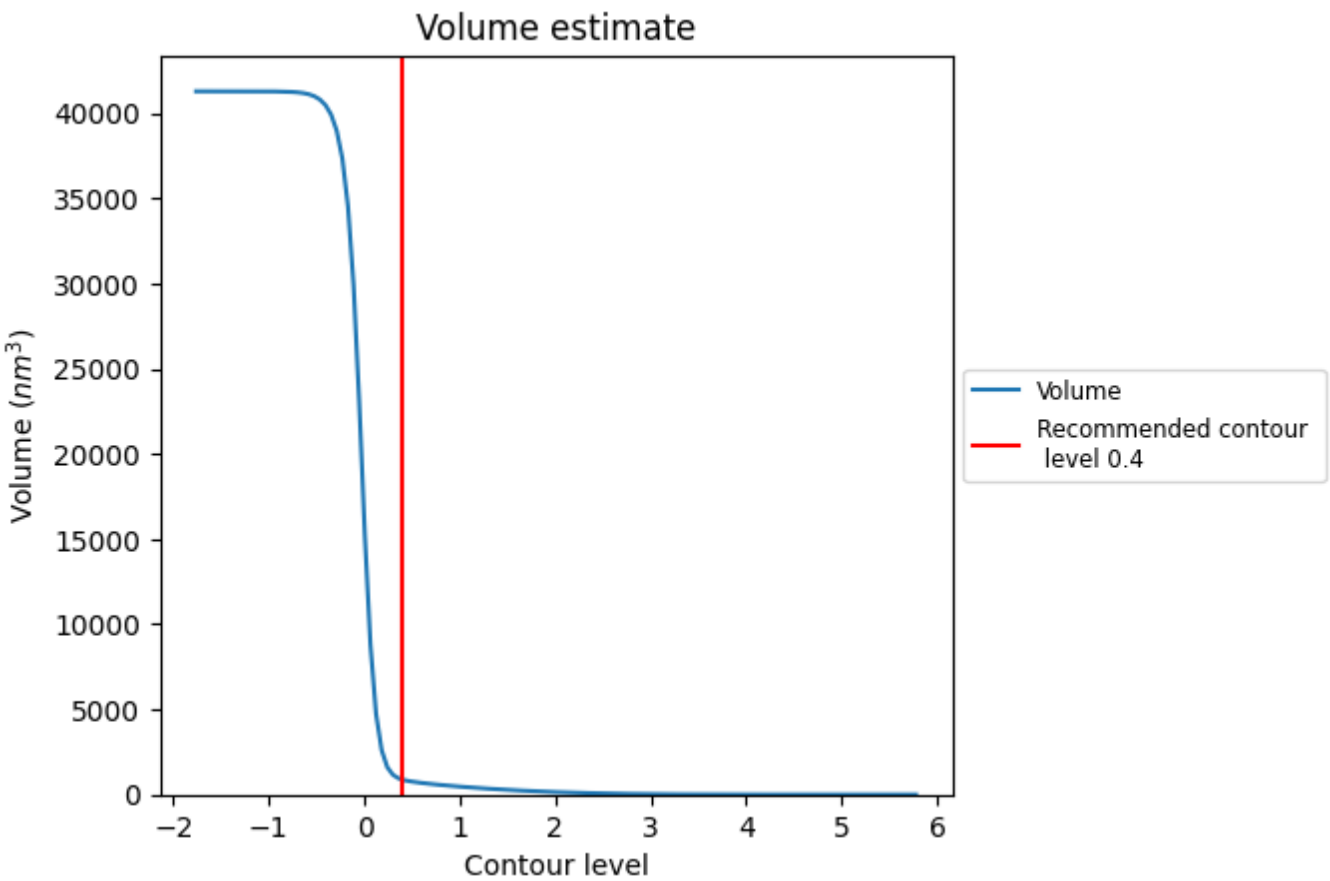
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

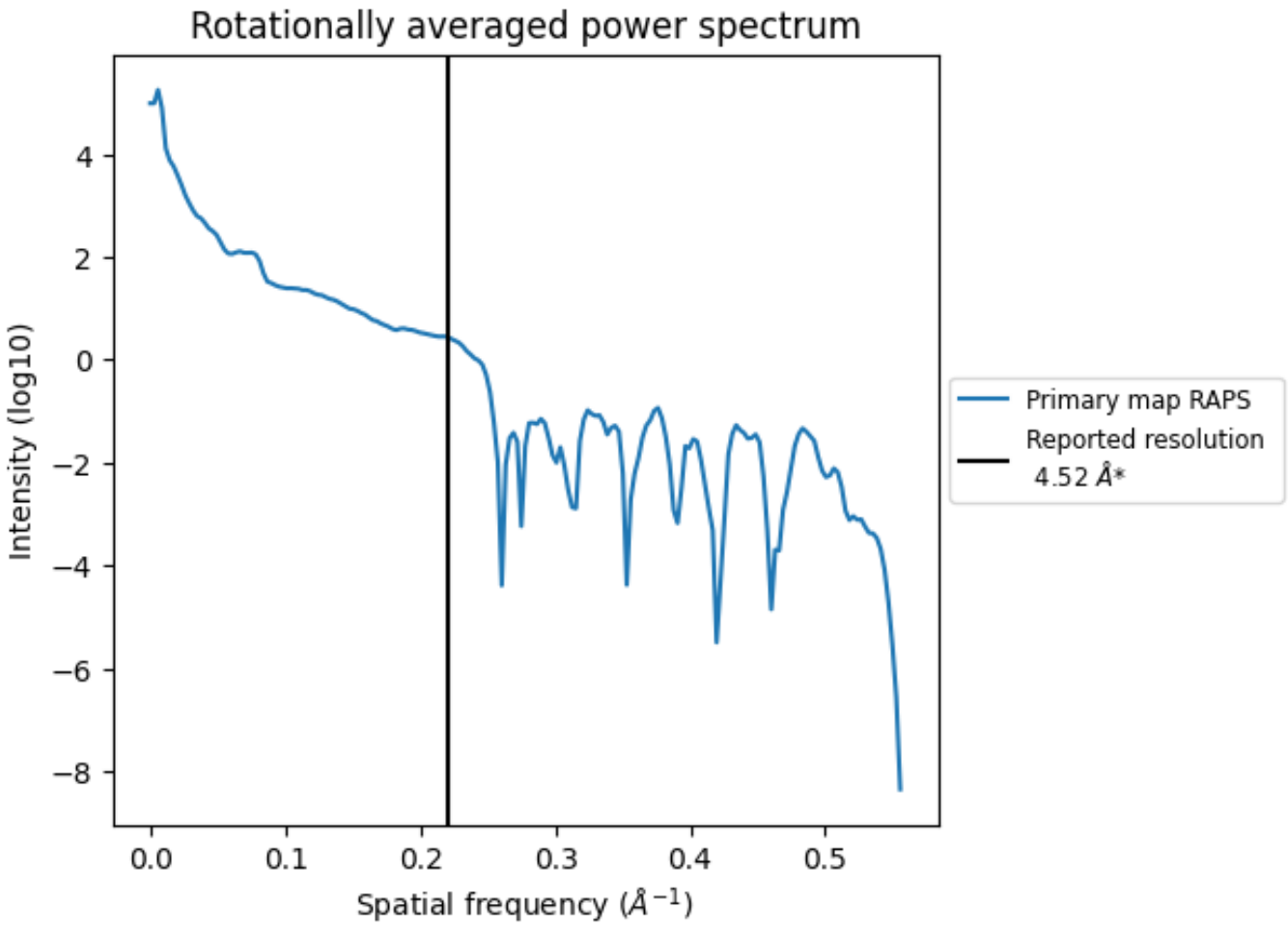
7.2 Volume estimate (i)



The volume at the recommended contour level is 881 nm^3; this corresponds to an approximate mass of 796 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 0.221 Å^{-1}

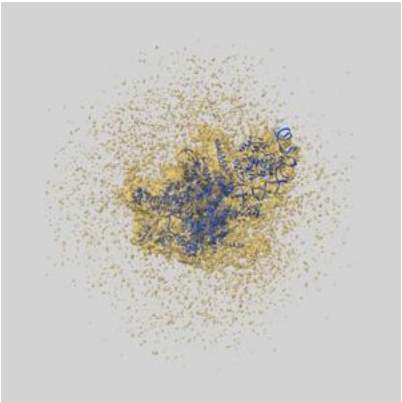
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

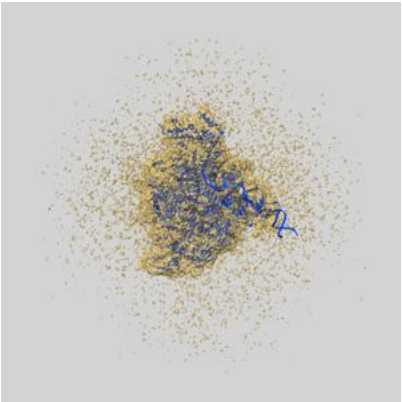
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20287 and PDB model 6PB5. Per-residue inclusion information can be found in section 3 on page 7.

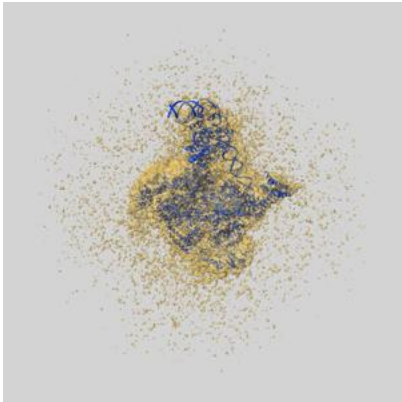
9.1 Map-model overlay (i)



X



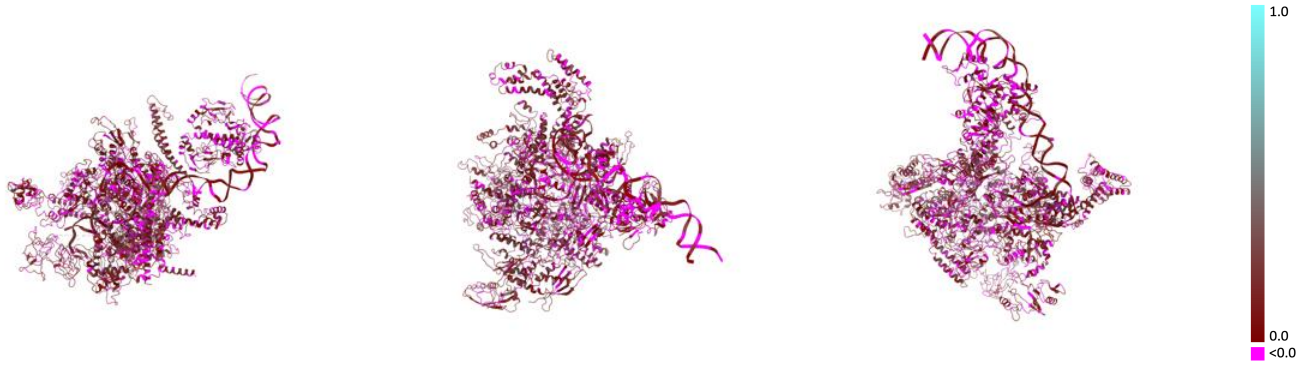
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

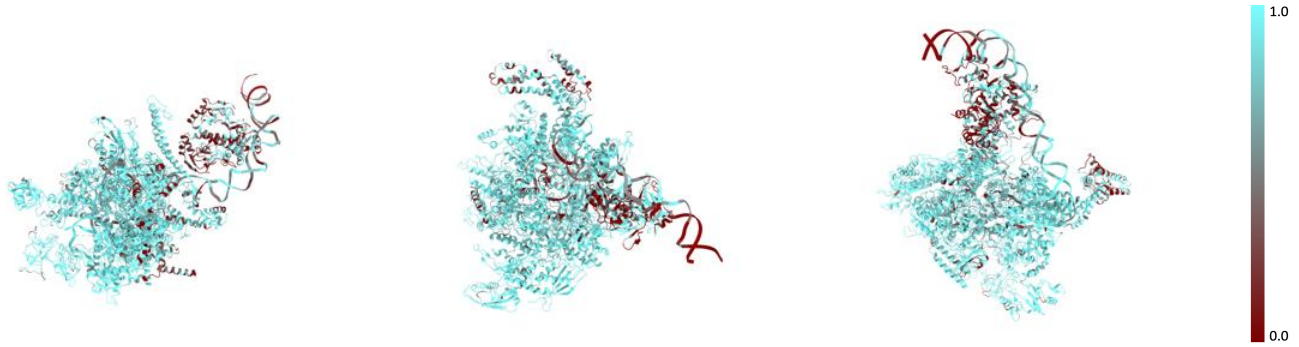
9.2 Q-score mapped to coordinate model (i)



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.

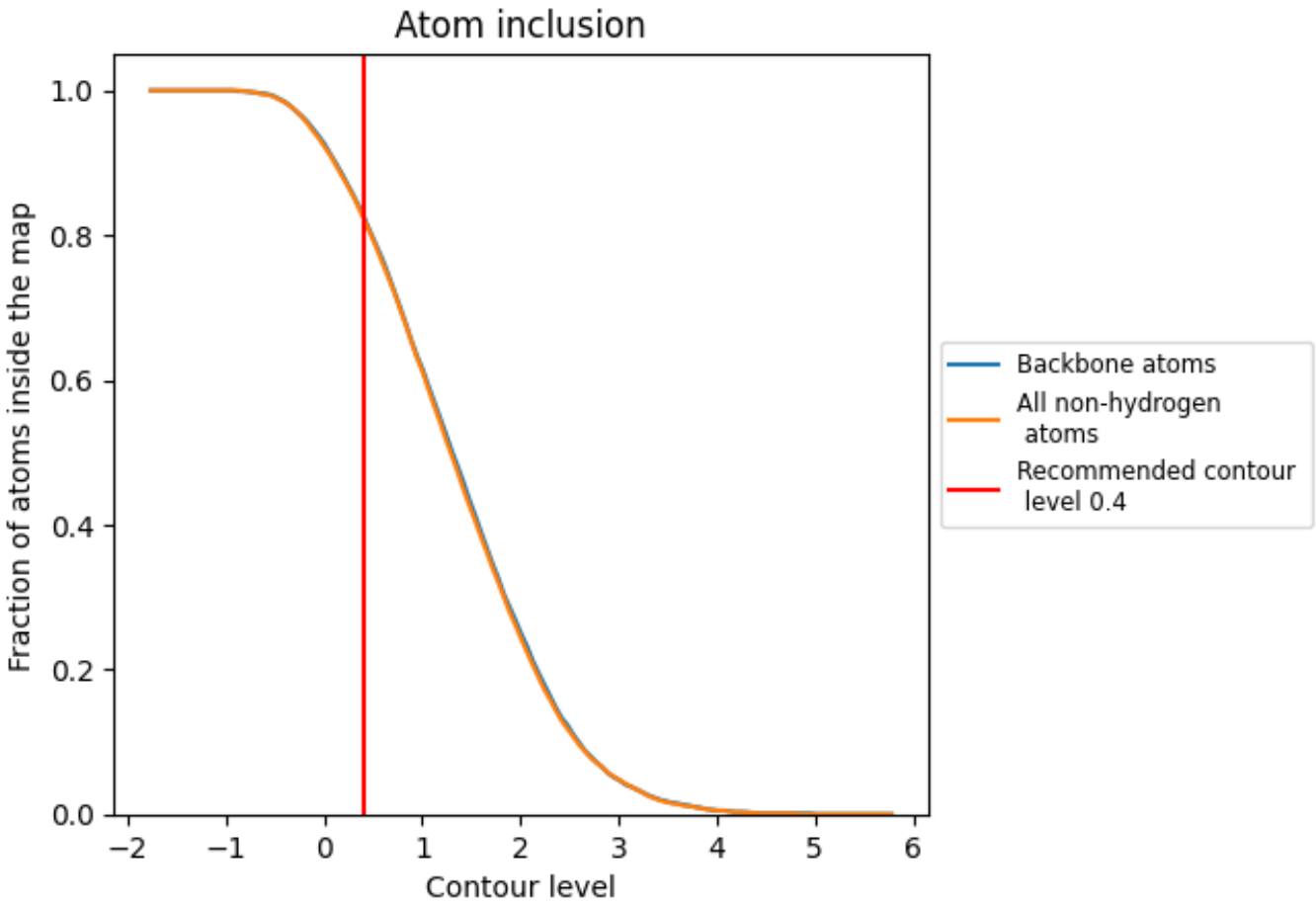
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.0820
1	0.6530	0.0640
2	0.6140	0.0680
A	0.9410	0.0860
B	0.9380	0.1250
C	0.8970	0.0740
D	0.9450	0.1100
E	0.6270	0.0430
F	0.7190	0.0700
G	0.3580	0.0280
H	0.4380	0.0200