wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:38 AM EST

PDB ID	:	7M7G
EMDB ID	:	EMD-23712
Title	:	6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 2
Authors	:	Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on	:	2021-03-28
Resolution	:	4.10 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

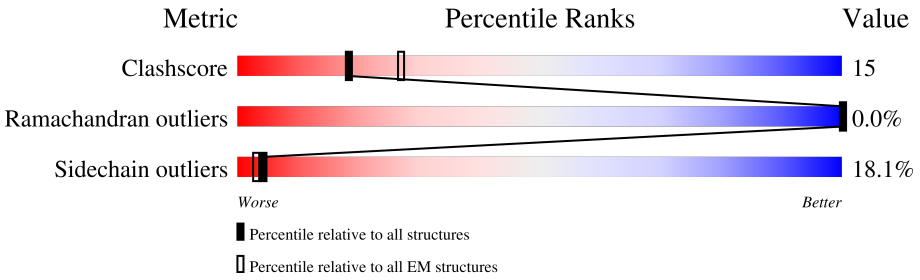
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.10 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	1784	23% 47% 26% · 24%
1	B	1784	20% 47% 26% · 23%
2	C	249	45% 30% 7% · 18%
2	E	249	· 43% 33% 6% 18%
3	D	236	· 45% 39% · 13%
3	F	236	· 45% 39% · · 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26480 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1356	Total	C	N	O	S	0	0
			10046	6244	1845	1922	35		
1	B	1379	Total	C	N	O	S	0	0
			10220	6356	1875	1954	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133

- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

- Molecule 3 is a protein called 1B2 (light chain).

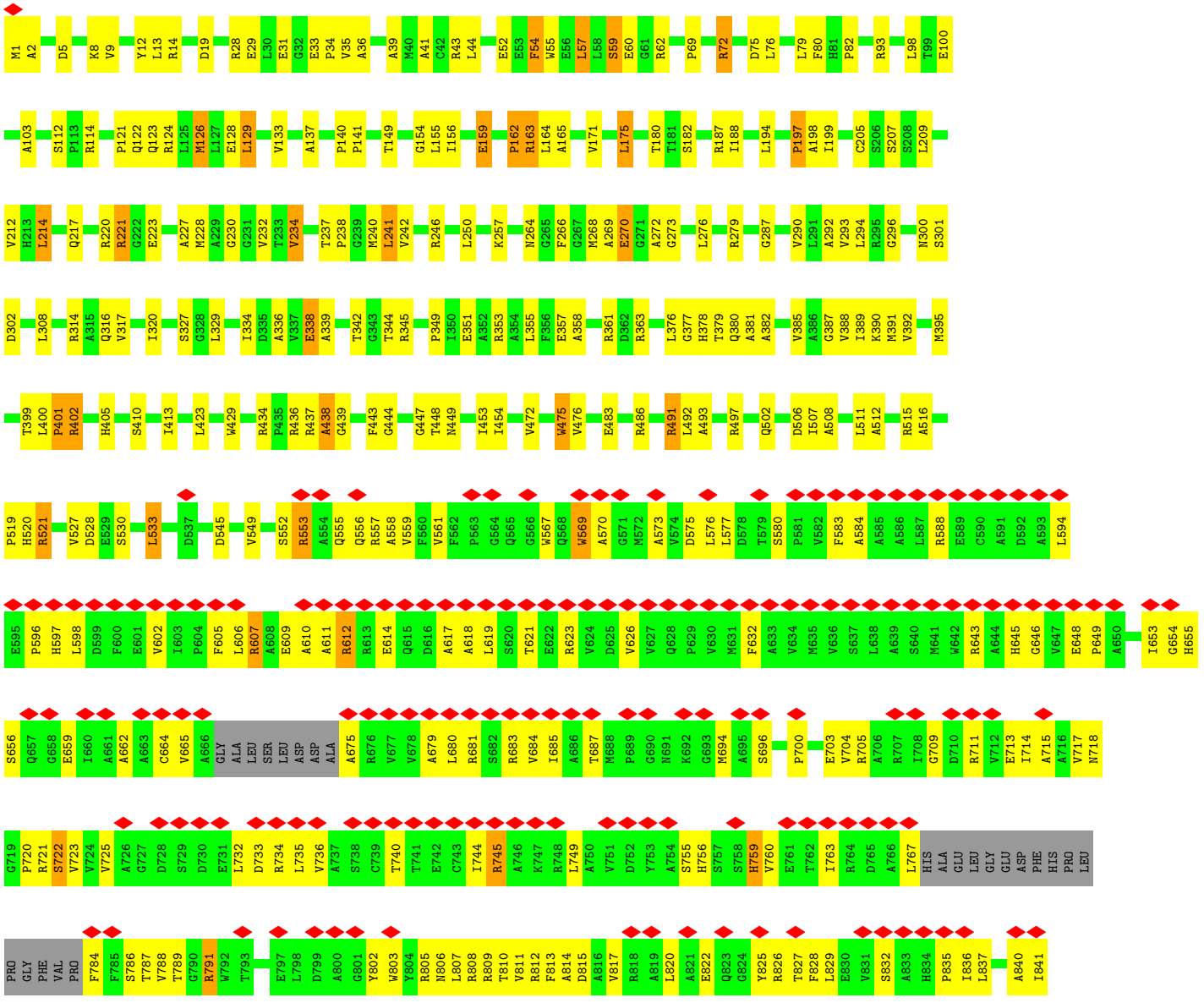
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

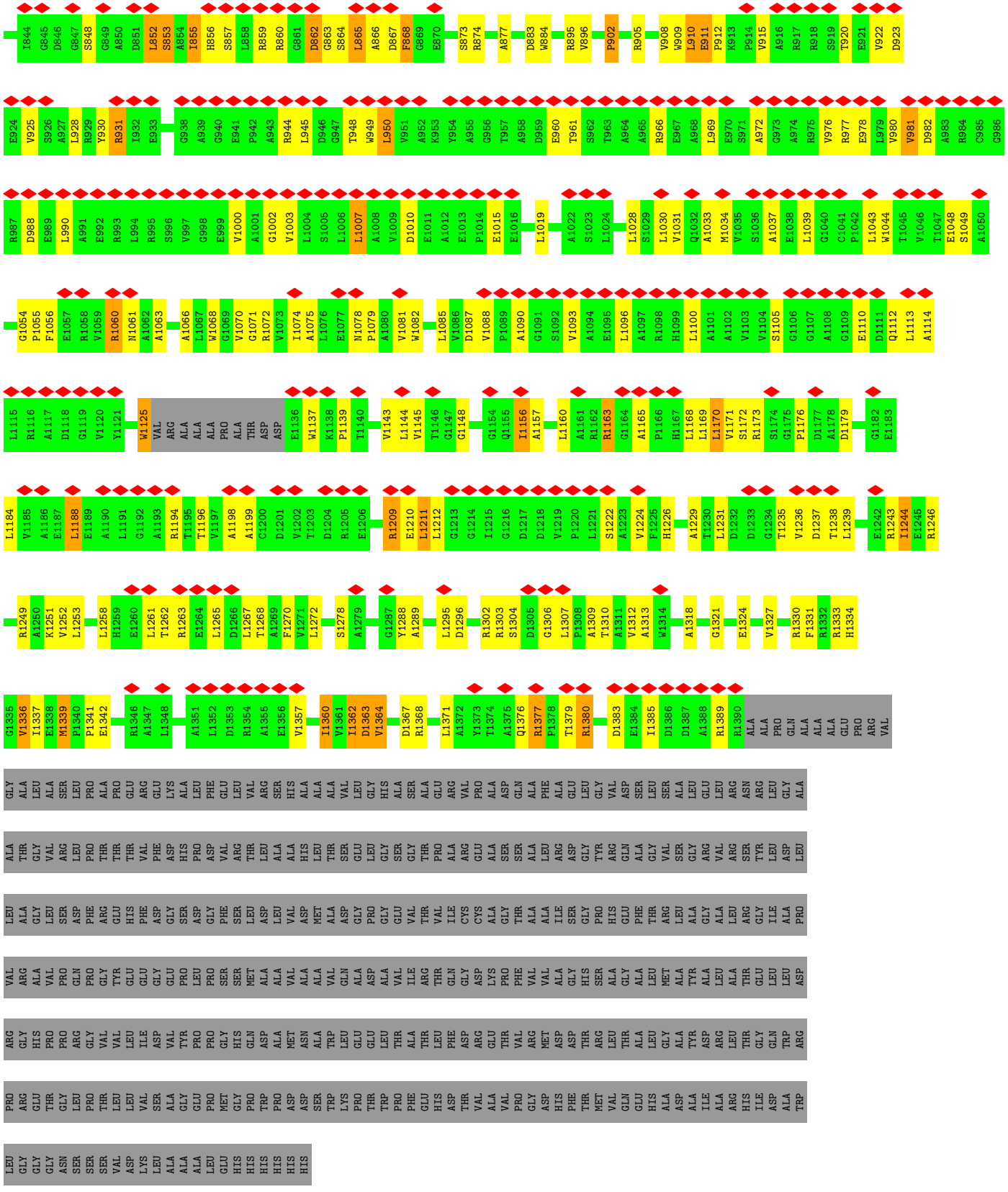
3 Residue-property plots (i)

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: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

Chain A:

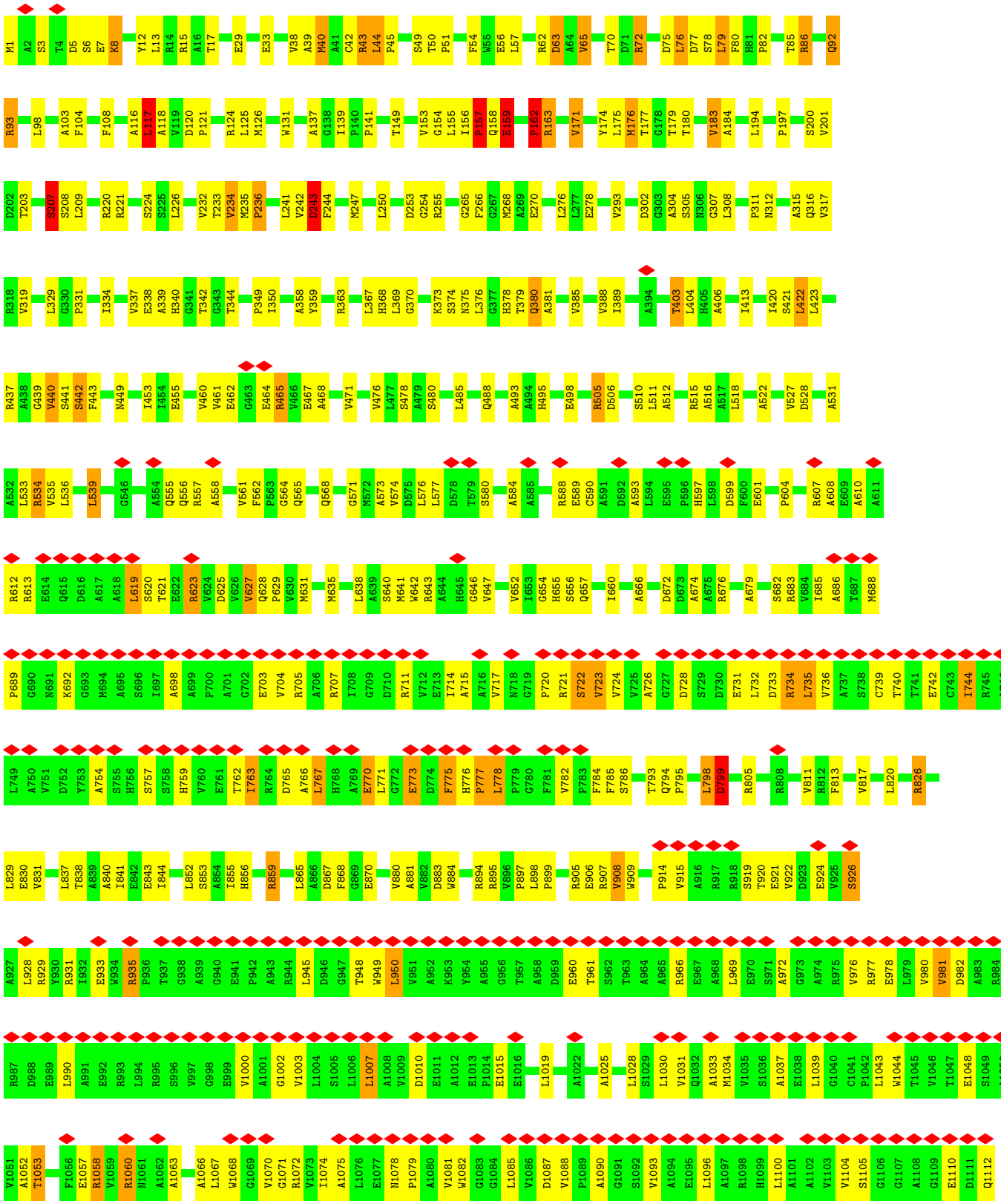


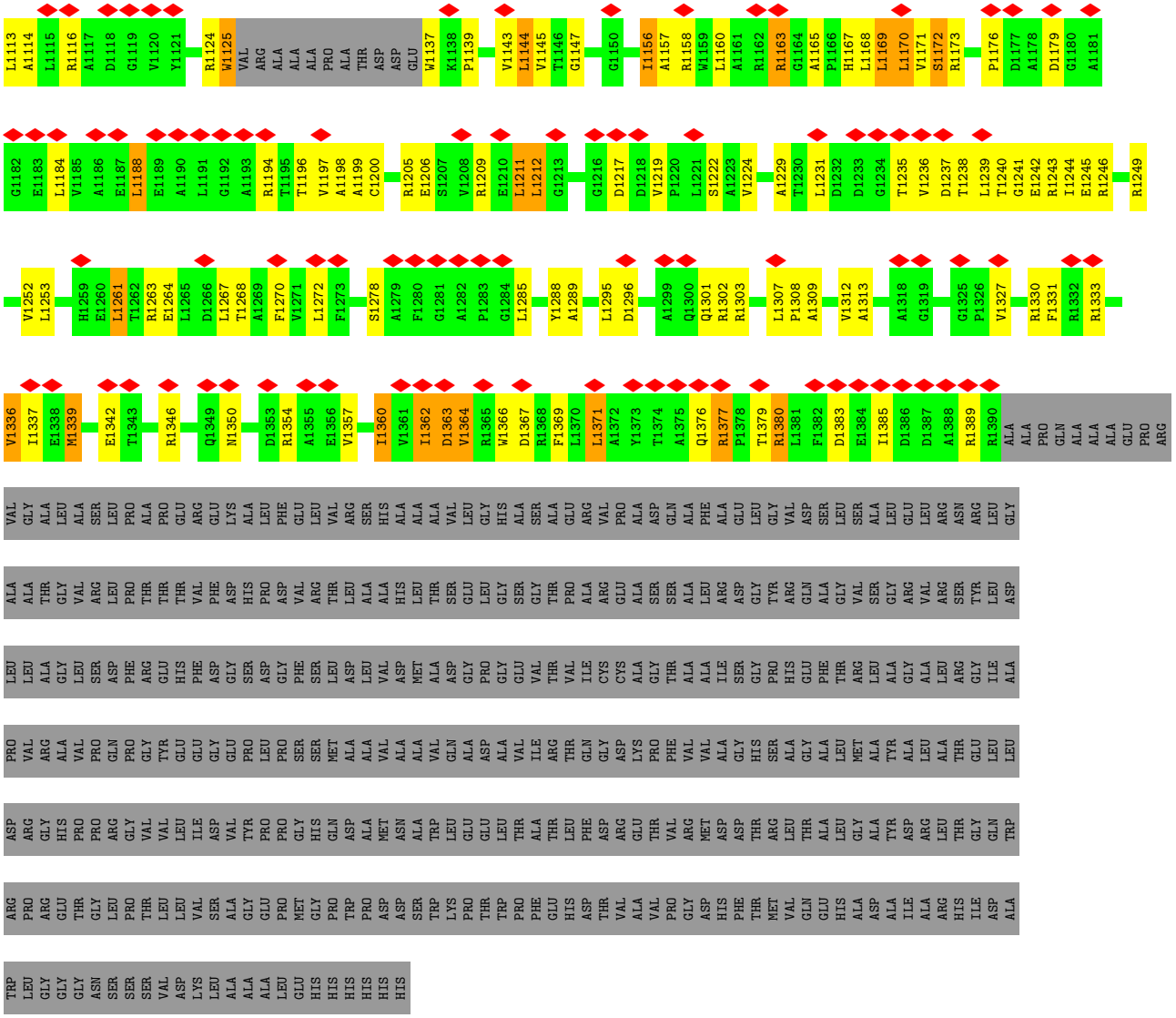


• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

Chain B:

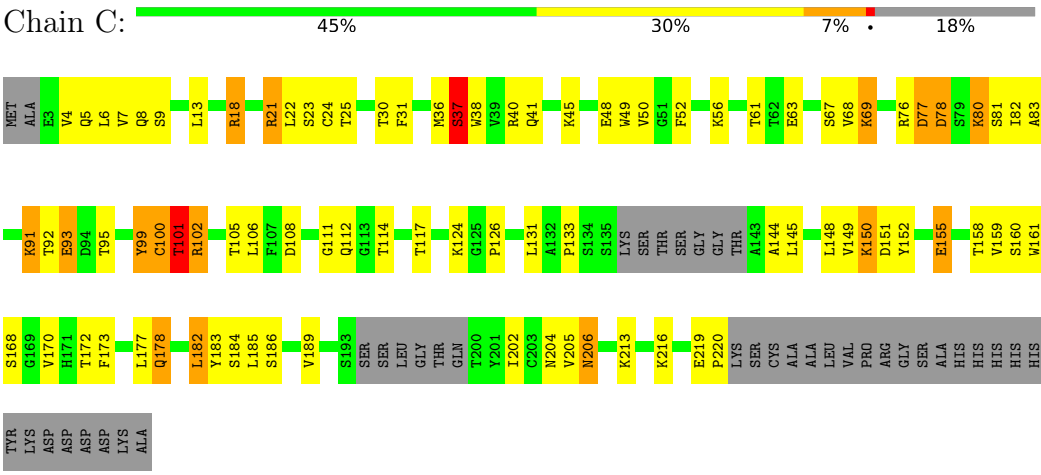

20%
47%
26%
23%


M1 A2 S3 T4 D5 S6 E7 K8 Y12 L13 R14 R15 A16 T17 E29 E33 V38 A39 M40 A41 C42 R43 L44 P45 S49 T50 P51 F54 W55 E56 L57 R62 D63 A64 V65 T70 D71 R72 D75 L76 D77 S78 L79 F80 H81 P82 T85 R86 Q92
R93 L98 A103 F104 F108 A116 L117 A118 V119 D120 P121 R124 L125 M126 W131 A137 G138 I139 P140 P141 T149 V153 G154 L155 I156 P157 Q158 E159 P162 R163 V171 Y174 L175 M176 T177 G178 T179 T180 V183 A184 L194 P197 S200 V201
D202 T203 S207 S208 L209 R220 R221 S224 S225 L226 V232 T233 V234 M235 P236 L241 V242 D243 F244 M247 L250 D253 G254 R255 G265 F266 G267 M268 A269 E270 L276 L277 E278 V293 D302 G303 A304 S305 N306 G307 L308 P311 N312 A315 Q316 V317
R318 V319 L329 G330 P331 I334 V337 E338 A339 H340 G341 T342 G343 T344 P349 I350 A358 Y359 R363 L367 H368 L369 G370 K373 S374 N375 L376 G377 H378 T379 Q380 A381 V385 V388 I389 A394 T403 L404 H405 A406 I413 I420 S421 L422 L423
R437 A438 G439 V440 S441 S442 F443 N449 I453 I454 E455 V460 V461 E462 G463 E464 R465 V466 E467 A468 V471 V476 L477 S478 A479 S480 L485 Q488 A493 A494 H495 E498 R505 D506 S510 L511 A512 R515 A516 A517 L518 A522 V527 D528 A531
A532 L533 R534 V535 L536 L539 G546 A554 Q555 Q556 R557 A558 V561 F562 P563 G564 Q565 Q568 G571 M572 A573 V574 D575 L576 L577 D578 T579 S580 A584 A585 R588 E589 C590 A591 D592 A593 L594 E595 P596 H597 L598 D599 F600 E601 P604 R607 A608 E609 A610 A611
R612 R613 E614 Q615 D616 A617 A618 L619 S620 T621 E622 R623 V624 D625 V626 V627 Q628 P629 V630 M631 M635 L638 A639 S640 M641 W642 R643 A644 H645 G646 V647 V652 I653 G654 H655 S656 Q657 I660 A666 D672 D673 A674 A675 R676 A679 S682 R683 V684 I685 A686 T687 M688
P689 G690 N691 K692 G693 M694 A695 S696 I697 A698 A699 P700 A701 G702 E703 V704 R705 A706 R707 I708 G709 D710 R711 V712 E713 I714 A715 A716 V717 N718 G719 P720 R721 S722 V723 V724 V725 A726 G727 D728 S729 D730 E731 L732 D733 R734 L735 V736 A737 S738 C739 T740 T741 E742 G743 I744 R745 A746 K747 R748
L749 A750 V751 D752 Y753 A754 S755 H756 S757 S758 H759 V760 E761 T762 I763 R764 D765 A766 L767 H768 A769 E770 L771 G772 E773 D774 F775 H776 P777 L778 P779 G780 F781 V782 P783 F784 F785 S786 T793 Q794 P795 L798 D799 R805 R808 V811 R812 F813 V817 L820 R826
L829 E830 V831 L837 T838 A839 A840 I841 E842 E843 I844 L852 S853 A854 I855 H856 R859 L865 A866 D867 F868 G869 E870 V880 A881 V882 D883 W884 R894 R895 V896 P897 L898 P899 R905 E906 R907 V908 W909 P914 V915 A916 R917 R918 S919 T920 E921 V922 D923 E924 V925 S926
A927 L928 R929 Y930 R931 I932 E933 W934 R935 P936 T937 G938 A939 G940 E941 P942 A943 R944 L945 D946 G947 T948 W949 L950 V951 A952 K953 Y954 A955 G956 T957 A958 D959 E960 T961 S962 T963 A964 A965 R966 E967 A968 L969 E970 S971 A972 G973 A974 R975 V976 R977 E978 L979 V980 V981 D982 A983 R984 C985 G986
R987 D988 E989 L990 A991 E992 R993 L994 R995 S996 V997 G998 E999 V1000 A1001 G1002 V1003 L1004 S1005 L1006 L1007 A1008 V1009 D1010 E1011 A1012 E1013 P1014 E1015 E1016 L1019 A1022 A1025 L1028 S1029 L1030 V1031 Q1032 A1033 M1034 V1035 S1036 A1037 E1038 L1039 G1040 C1041 P1042 L1043 W1044 T1045 V1046 T1047 E1048 S1049 A1050
V1051 A1052 T1053 F1056 E1057 R1058 V1059 R1060 N1061 A1062 A1063 A1066 L1067 W1068 G1069 V1070 G1071 R1072 V1073 I1074 A1075 L1076 E1077 N1078 P1079 A1080 V1081 W1082 G1083 G1084 L1085 V1086 D1087 V1088 P1089 A1090 G1091 S1092 V1093 A1094 E1095 L1096 A1097 R1098 H1099 L1100 A1101 A1102 V1103 V1104 S1105 G1106 G1107 A1108 G1109 E1110 D1111 Q1112



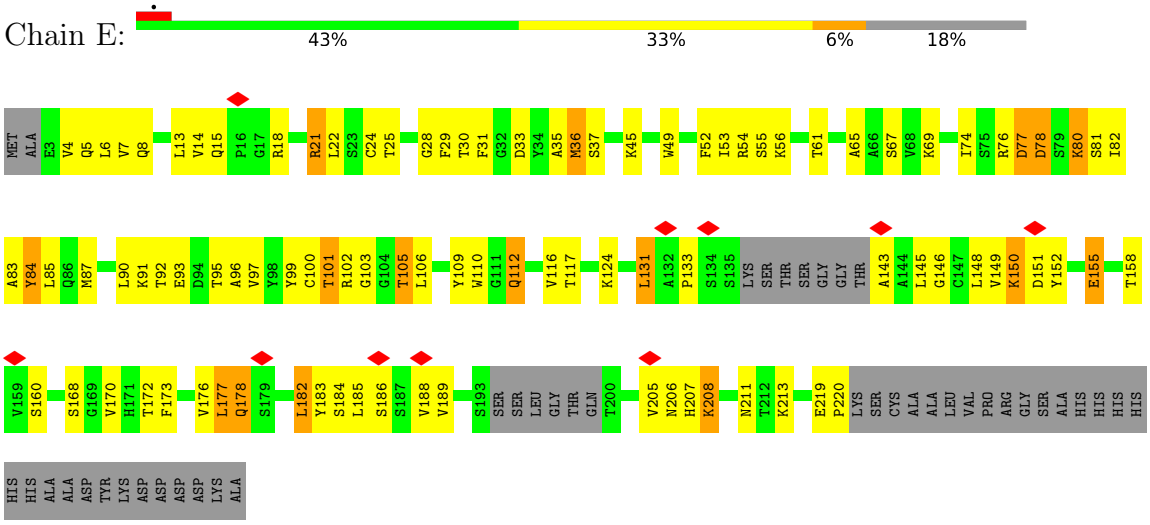
• Molecule 2: 1B2 (heavy chain)

Chain C:



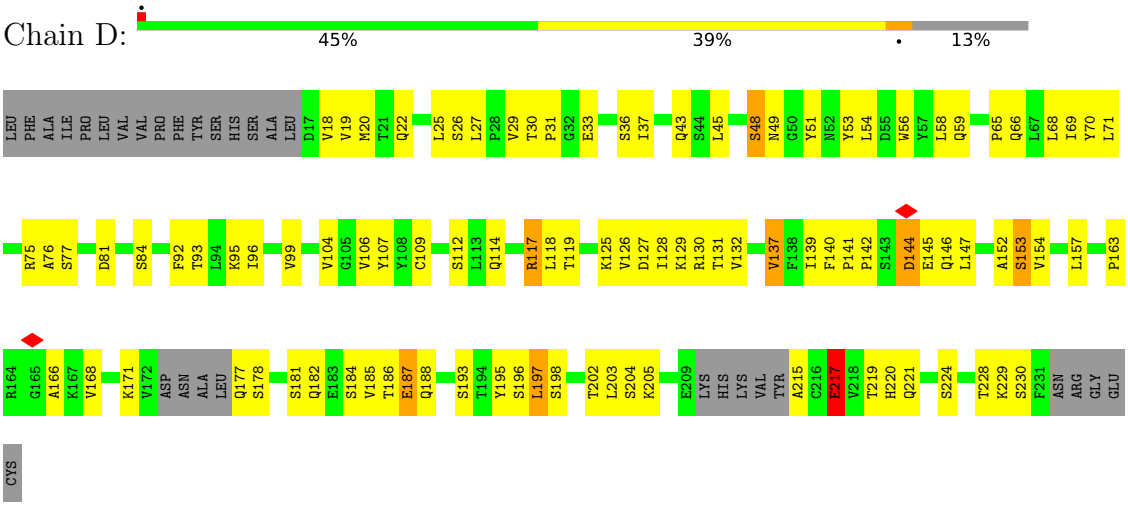
• Molecule 2: 1B2 (heavy chain)

Chain E:



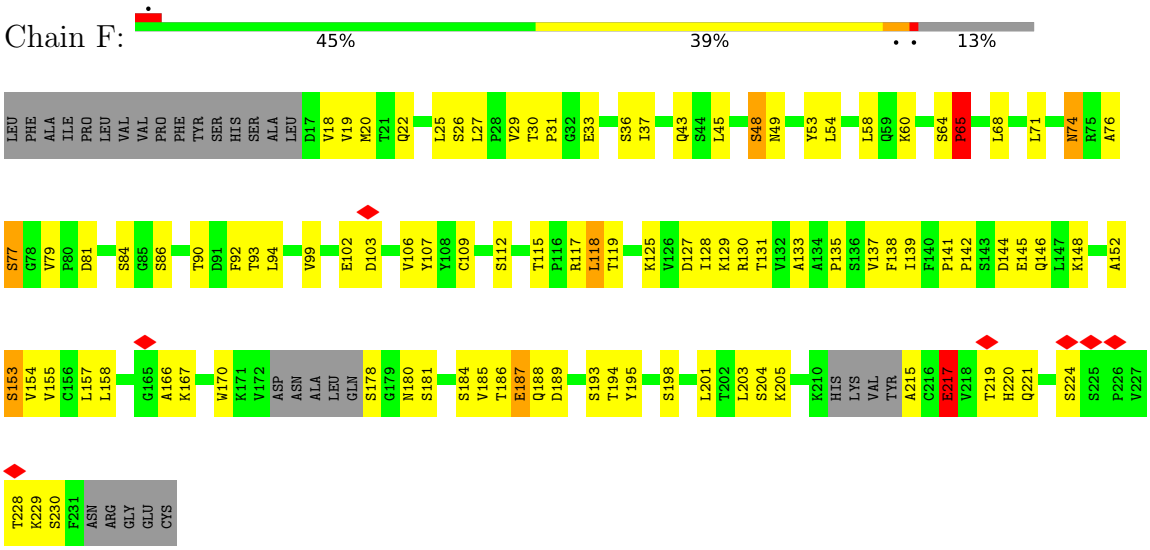
• Molecule 3: 1B2 (light chain)

Chain D:



• Molecule 3: 1B2 (light chain)

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.610	Depositor
Minimum map value	-1.457	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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	0.63	19/10238 (0.2%)	0.79	27/13933 (0.2%)
1	B	0.66	19/10421 (0.2%)	0.82	20/14187 (0.1%)
2	C	0.62	3/1575 (0.2%)	0.86	5/2141 (0.2%)
2	E	0.58	1/1575 (0.1%)	0.84	3/2141 (0.1%)
3	D	0.46	1/1601 (0.1%)	0.68	1/2175 (0.0%)
3	F	0.57	3/1601 (0.2%)	0.80	6/2174 (0.3%)
All	All	0.63	46/27011 (0.2%)	0.80	62/36751 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
2	C	0	2
2	E	0	3
3	F	0	1
All	All	0	9

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	SER	CA-CB	-16.16	1.28	1.52
1	B	442	SER	CA-CB	-14.70	1.30	1.52
1	B	441	SER	CA-CB	-10.75	1.36	1.52
1	A	230	GLY	C-O	-8.66	1.09	1.23
1	A	197	PRO	C-O	-8.28	1.06	1.23

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	PRO	N-CA-CB	-16.52	83.47	103.30
1	B	159	GLU	CB-CA-C	-16.13	78.14	110.40
1	B	157	PRO	N-CA-CB	-12.40	88.42	103.30
2	C	102	ARG	CB-CA-C	-10.26	89.89	110.40
2	E	102	ARG	CB-CA-C	-10.24	89.92	110.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ASP	Mainchain
1	B	171	VAL	Mainchain
1	B	799	ASP	Sidechain
2	C	155	GLU	Peptide
2	C	21	ARG	Sidechain

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	10046	0	9883	279	0
1	B	10220	0	10049	293	0
2	C	1539	0	1511	61	0
2	E	1539	0	1511	62	0
3	D	1568	0	1528	52	0
3	F	1568	0	1533	54	0
All	All	26480	0	26015	764	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 15.

The worst 5 of 764 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:PRO:HG3	1:B:799:ASP:CG	1.62	1.18
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ALA:HB2	1:A:863:GLY:HA2	1.57	0.85
1:B:777:PRO:HG3	1:B:799:ASP:OD2	1.87	0.73
1:A:610:ALA:HB3	1:A:862:ASP:HB2	1.73	0.70

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	1348/1784 (76%)	1233 (92%)	114 (8%)	1 (0%)	51	84
1	B	1375/1784 (77%)	1243 (90%)	132 (10%)	0	100	100
2	C	199/249 (80%)	177 (89%)	22 (11%)	0	100	100
2	E	199/249 (80%)	175 (88%)	24 (12%)	0	100	100
3	D	200/236 (85%)	185 (92%)	15 (8%)	0	100	100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
All	All	3521/4538 (78%)	3200 (91%)	320 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	656	SER

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	999/1325 (75%)	840 (84%)	159 (16%)	2 15
1	B	1017/1325 (77%)	829 (82%)	188 (18%)	1 10
2	C	170/203 (84%)	132 (78%)	38 (22%)	1 6
2	E	170/203 (84%)	137 (81%)	33 (19%)	1 9
3	D	182/208 (88%)	146 (80%)	36 (20%)	1 8
3	F	182/208 (88%)	145 (80%)	37 (20%)	1 7
All	All	2720/3472 (78%)	2229 (82%)	491 (18%)	4 11

5 of 491 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	731	GLU
2	E	145	LEU
1	B	1010	ASP
2	E	97	VAL
3	F	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	86	GLN
2	C	112	GLN
3	F	188	GLN
3	D	188	GLN
1	B	1350	ASN

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)

There are no ligands in this entry.

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.

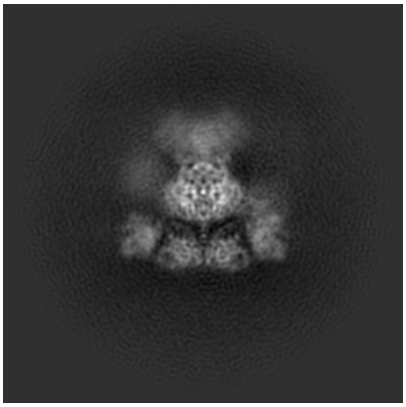
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23712. These allow visual inspection of the internal detail of the map and identification of artifacts.

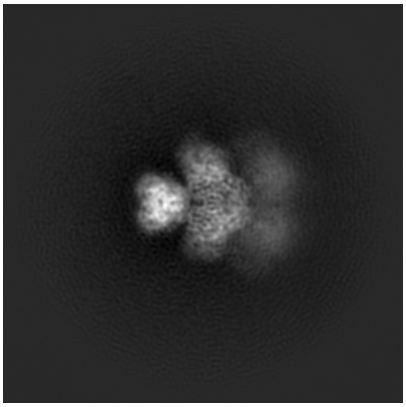
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

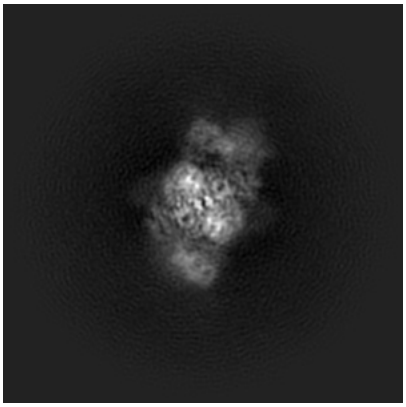
6.1.1 Primary map



X



Y

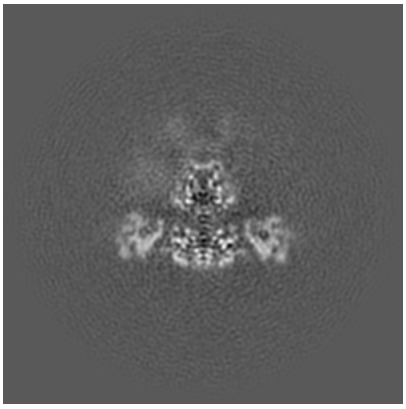


Z

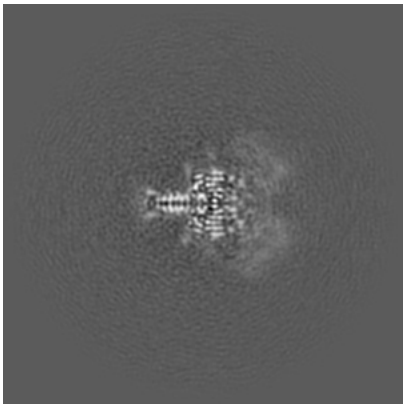
The images above show the map projected in three orthogonal directions.

6.2 Central slices

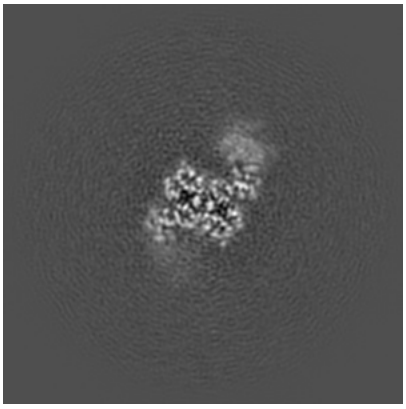
6.2.1 Primary map



X Index: 168



Y Index: 168

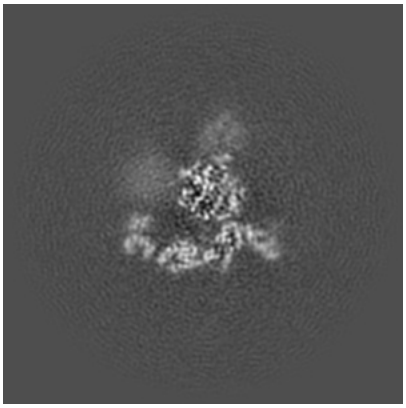


Z Index: 168

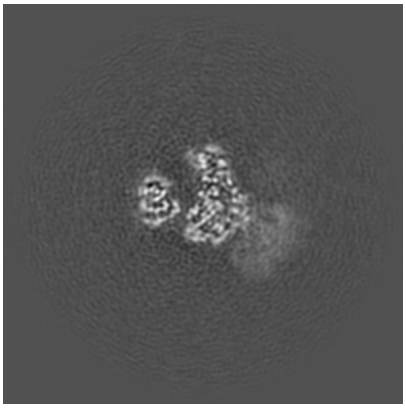
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

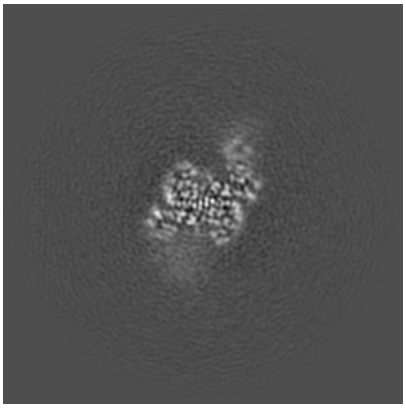
6.3.1 Primary map



X Index: 157



Y Index: 182

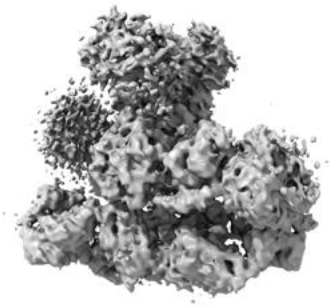


Z Index: 177

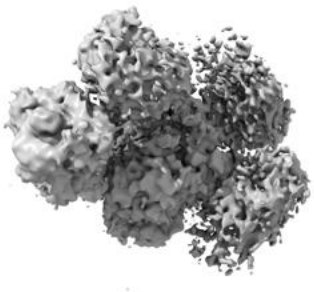
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

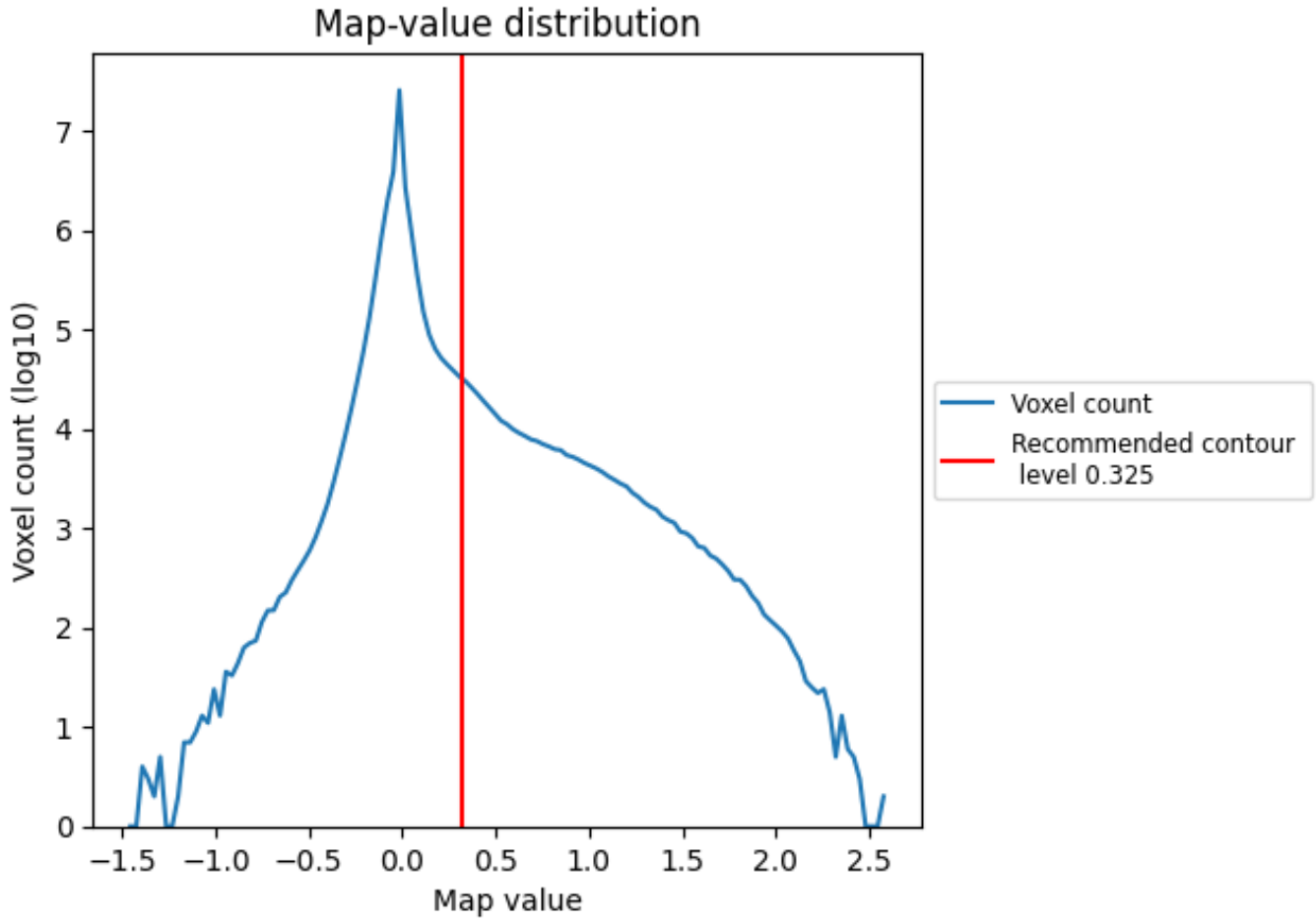
6.5 Mask visualisation (i)

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

7 Map analysis

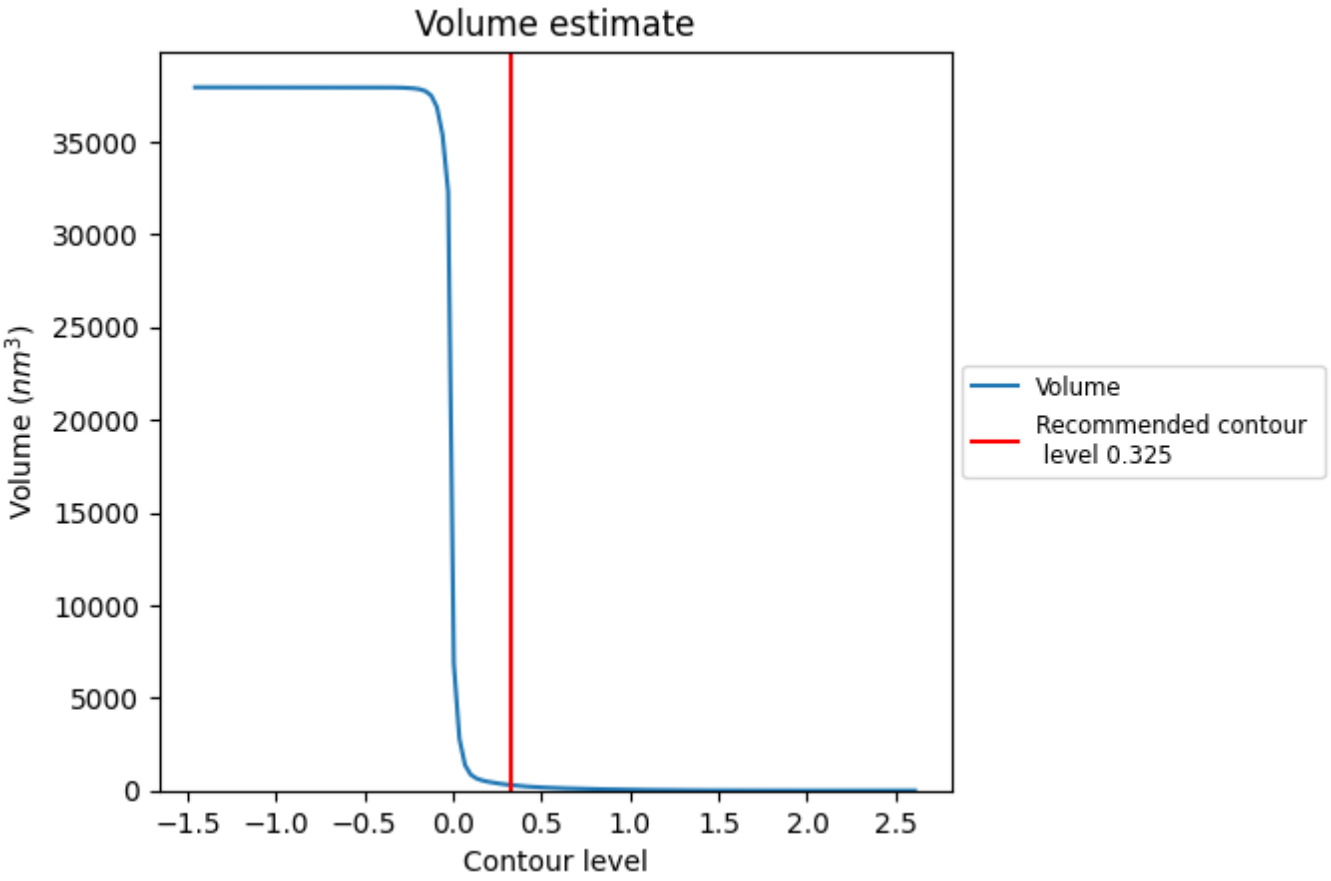
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

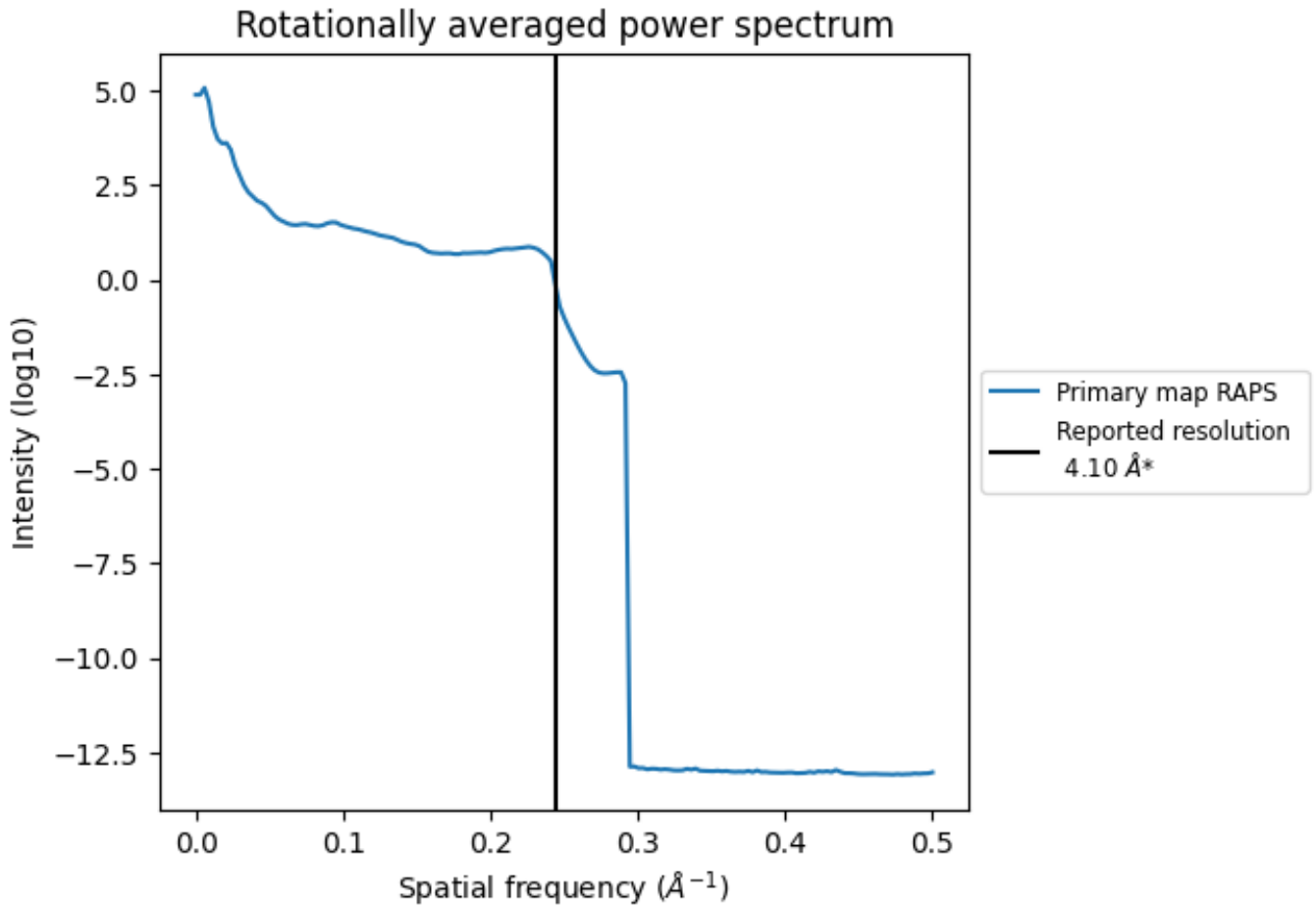
7.2 Volume estimate (i)



The volume at the recommended contour level is 299 nm^3; this corresponds to an approximate mass of 270 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 0.244 $Å^{-1}$

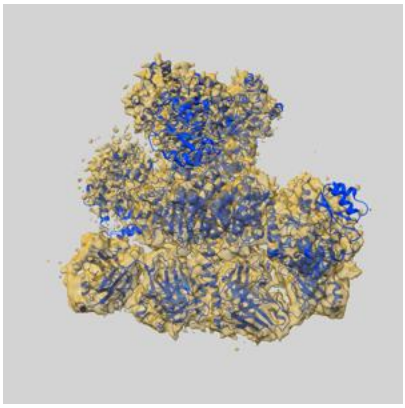
8 Fourier-Shell correlation (i)

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

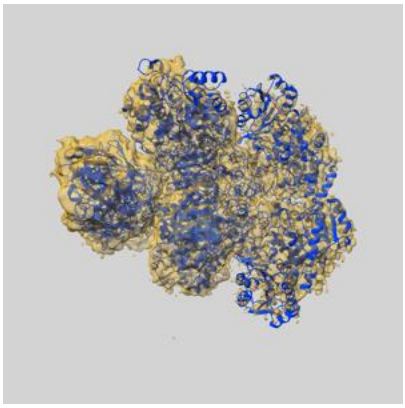
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23712 and PDB model 7M7G. Per-residue inclusion information can be found in section 3 on page 7.

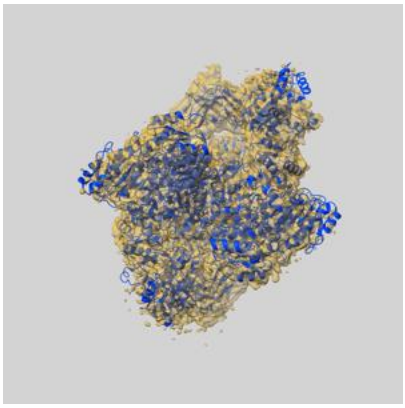
9.1 Map-model overlay



X



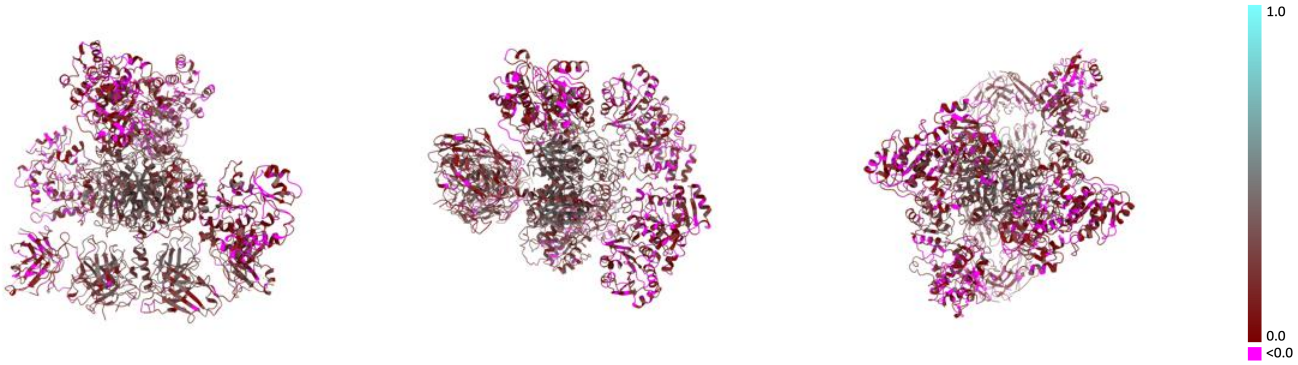
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.325 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.

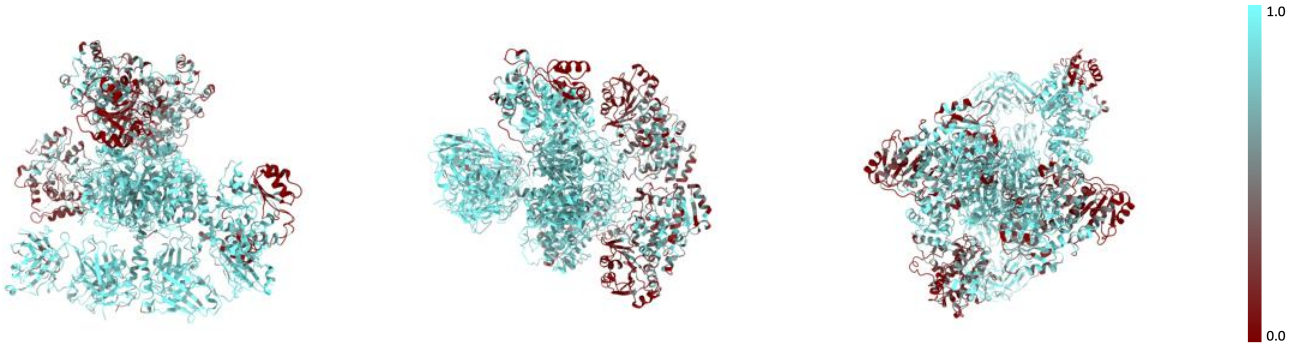
9.2 Q-score mapped to coordinate model (i)



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.

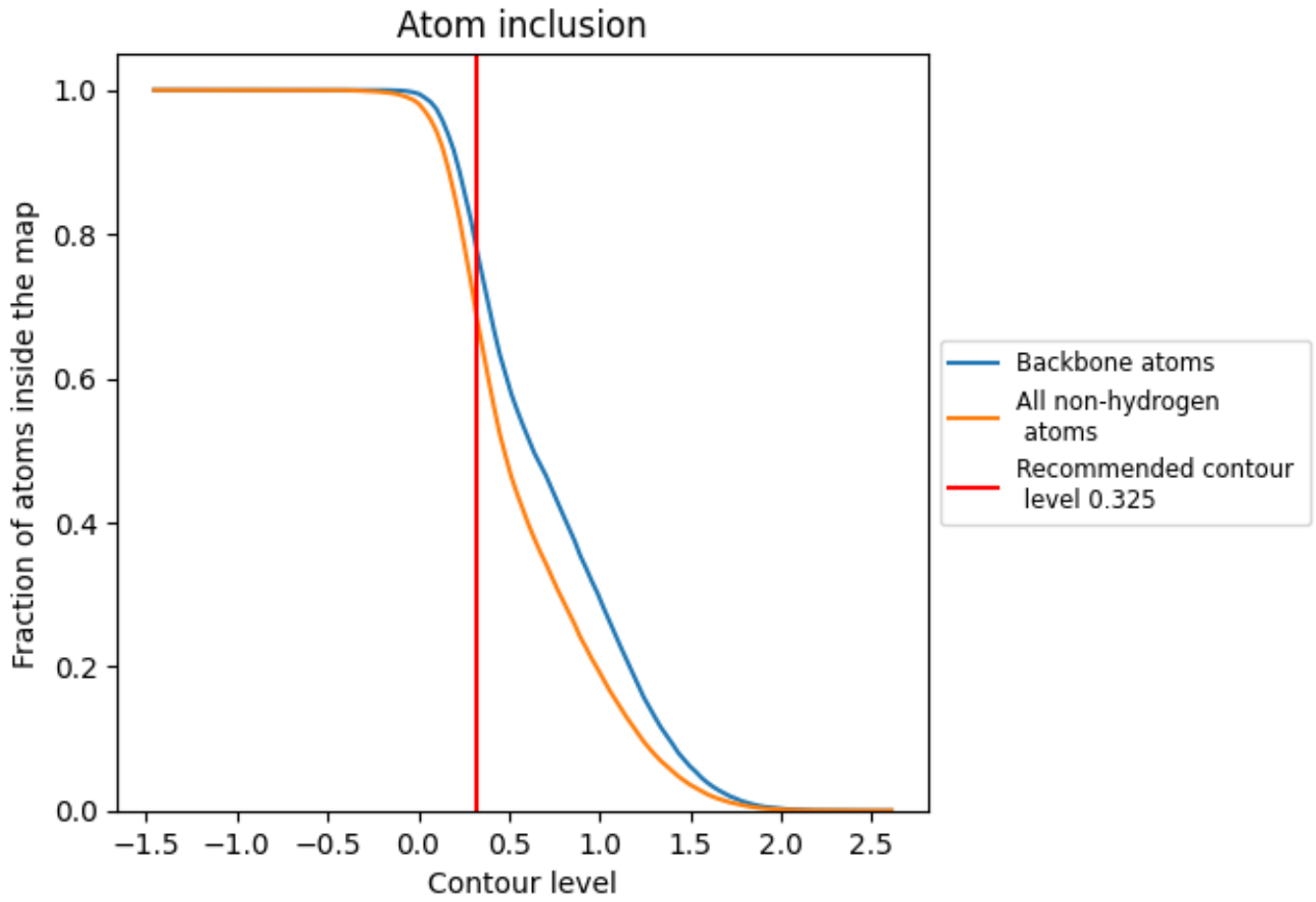
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.325).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6812	0.1810
A	0.6042	0.1680
B	0.6462	0.1690
C	0.8676	0.2240
D	0.8710	0.2570
E	0.8584	0.1780
F	0.8483	0.2210