wwPDB EM Validation Summary Report (i)

May 19, 2024 – 11:05 PM JST

PDB ID	:	7CPY
EMDB ID	:	EMD-30435
Title	:	Lovastatin nonaketide synthase with LovC
Authors	:	Wang, J.; Wang, Z.
Deposited on	:	2020-08-08
Resolution	:	3.60 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 (i)) were used in the production of this report:

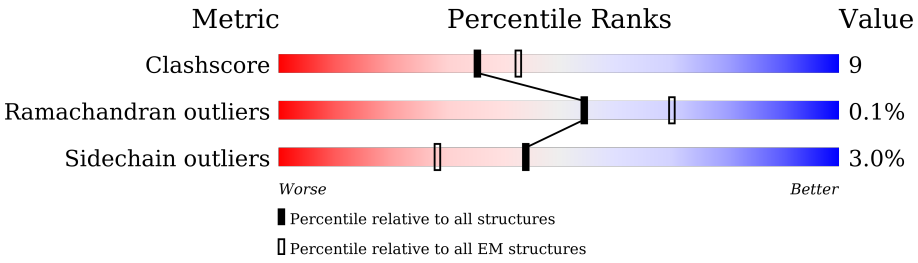
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

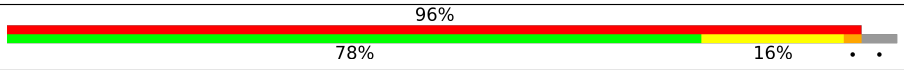
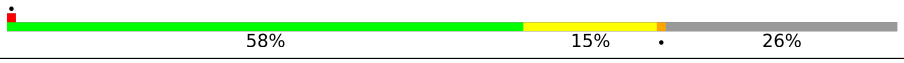
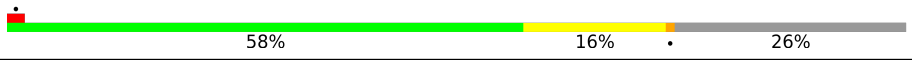
The reported resolution of this entry is 3.60 Å.

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	C	371	
1	D	371	
2	A	3046	
2	B	3046	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 75606 atoms, of which 34722 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 Lovastatin nonaketide synthase, enoyl reductase component lovC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	357	Total	C	N	O	S	0	0
			2742	1738	480	511	13		
1	D	357	Total	C	N	O	S	0	0
			2742	1738	480	511	13		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	364	LEU	-	expression tag	UNP Q9Y7D0
C	365	GLU	-	expression tag	UNP Q9Y7D0
C	366	HIS	-	expression tag	UNP Q9Y7D0
C	367	HIS	-	expression tag	UNP Q9Y7D0
C	368	HIS	-	expression tag	UNP Q9Y7D0
C	369	HIS	-	expression tag	UNP Q9Y7D0
C	370	HIS	-	expression tag	UNP Q9Y7D0
C	371	HIS	-	expression tag	UNP Q9Y7D0
D	364	LEU	-	expression tag	UNP Q9Y7D0
D	365	GLU	-	expression tag	UNP Q9Y7D0
D	366	HIS	-	expression tag	UNP Q9Y7D0
D	367	HIS	-	expression tag	UNP Q9Y7D0
D	368	HIS	-	expression tag	UNP Q9Y7D0
D	369	HIS	-	expression tag	UNP Q9Y7D0
D	370	HIS	-	expression tag	UNP Q9Y7D0
D	371	HIS	-	expression tag	UNP Q9Y7D0

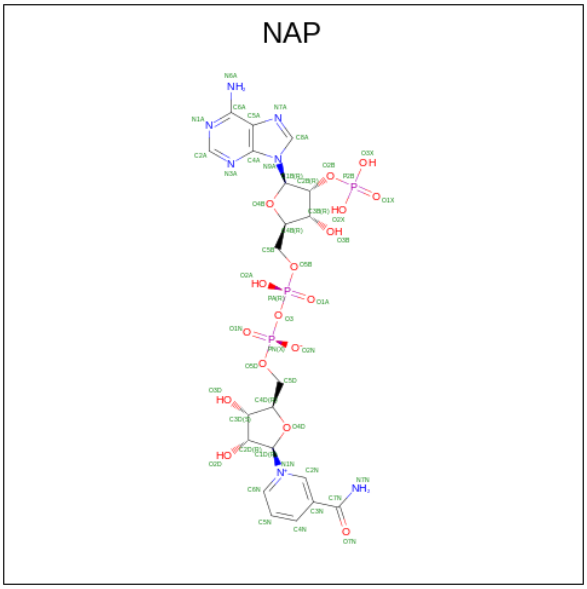
- Molecule 2 is a protein called Lovastatin nonaketide synthase, polyketide synthase component.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	2262	Total	C	H	N	O	S	0	0
			34988	11177	17336	3061	3325	89		
2	B	2262	Total	C	H	N	O	S	0	0
			34988	11177	17336	3061	3325	89		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
A	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
A	3039	HIS	-	expression tag	UNP Q9Y8A5
A	3040	VAL	-	expression tag	UNP Q9Y8A5
A	3041	HIS	-	expression tag	UNP Q9Y8A5
A	3042	HIS	-	expression tag	UNP Q9Y8A5
A	3043	HIS	-	expression tag	UNP Q9Y8A5
A	3044	HIS	-	expression tag	UNP Q9Y8A5
A	3045	HIS	-	expression tag	UNP Q9Y8A5
A	3046	HIS	-	expression tag	UNP Q9Y8A5
B	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
B	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
B	3039	HIS	-	expression tag	UNP Q9Y8A5
B	3040	VAL	-	expression tag	UNP Q9Y8A5
B	3041	HIS	-	expression tag	UNP Q9Y8A5
B	3042	HIS	-	expression tag	UNP Q9Y8A5
B	3043	HIS	-	expression tag	UNP Q9Y8A5
B	3044	HIS	-	expression tag	UNP Q9Y8A5
B	3045	HIS	-	expression tag	UNP Q9Y8A5
B	3046	HIS	-	expression tag	UNP Q9Y8A5

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



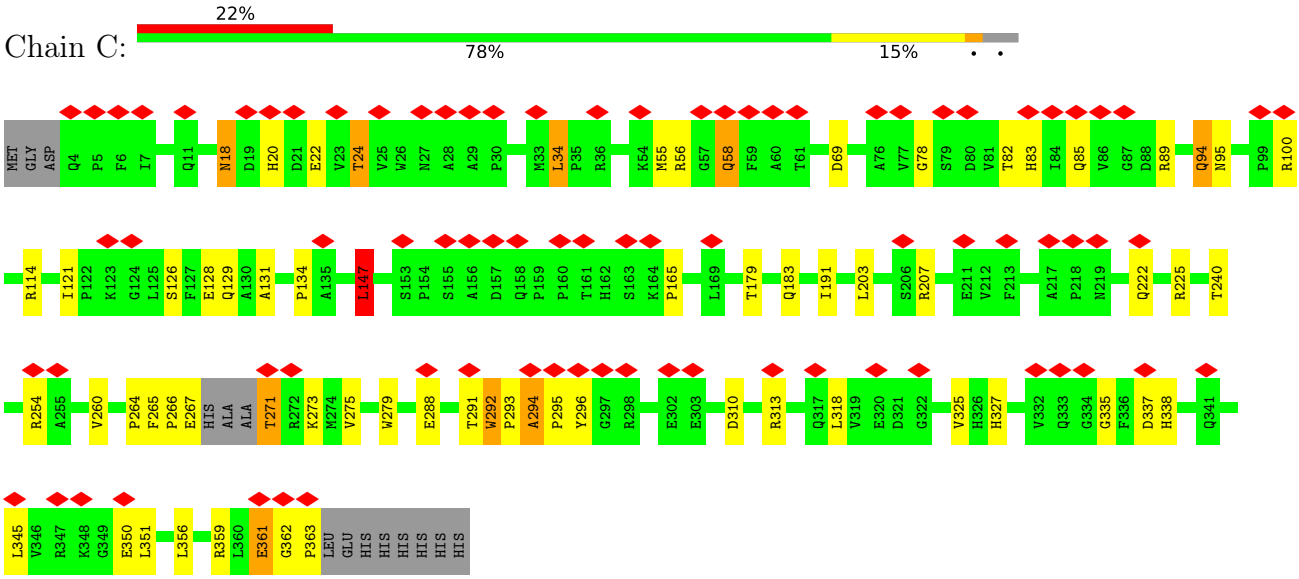
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			73	21	25	7	17	3	
3	B	1	Total	C	H	N	O	P	0
			73	21	25	7	17	3	

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.

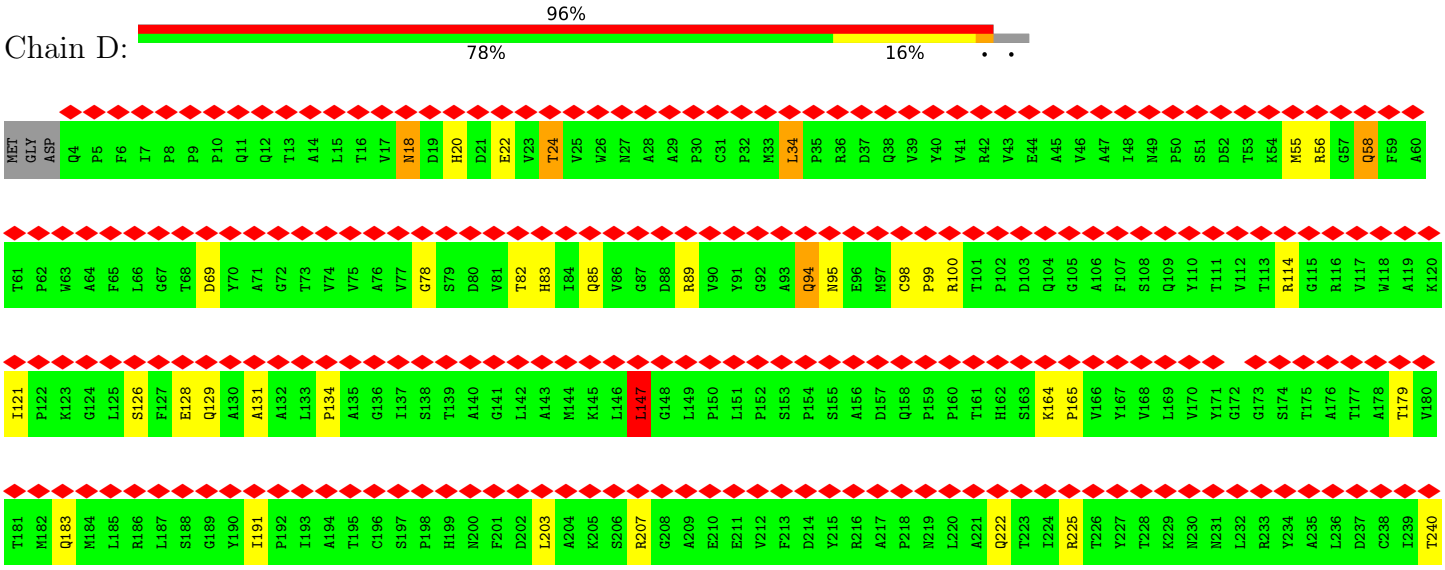
• Molecule 1: Lovastatin nonaketide synthase, enoyl reductase component lovC

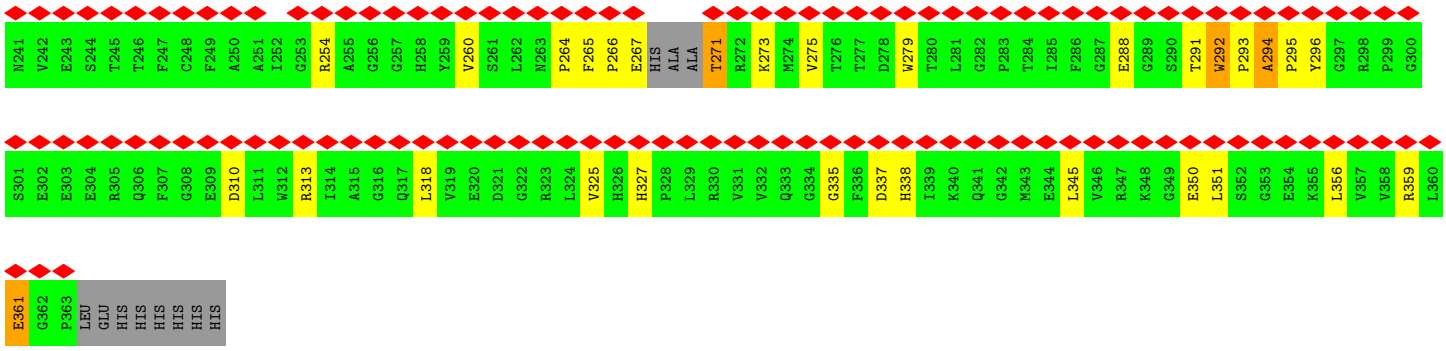
Chain C:



• Molecule 1: Lovastatin nonaketide synthase, enoyl reductase component lovC

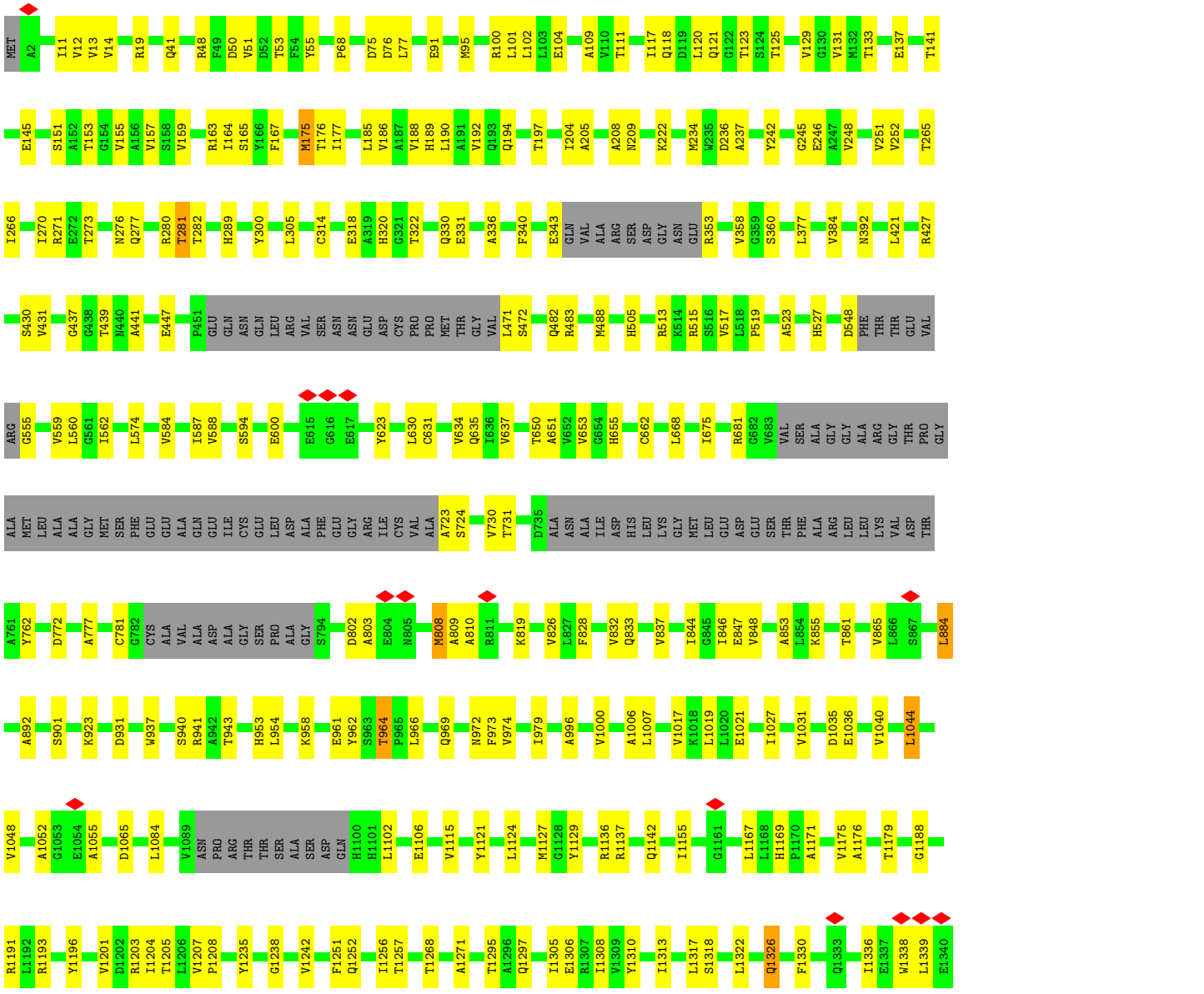
Chain D:

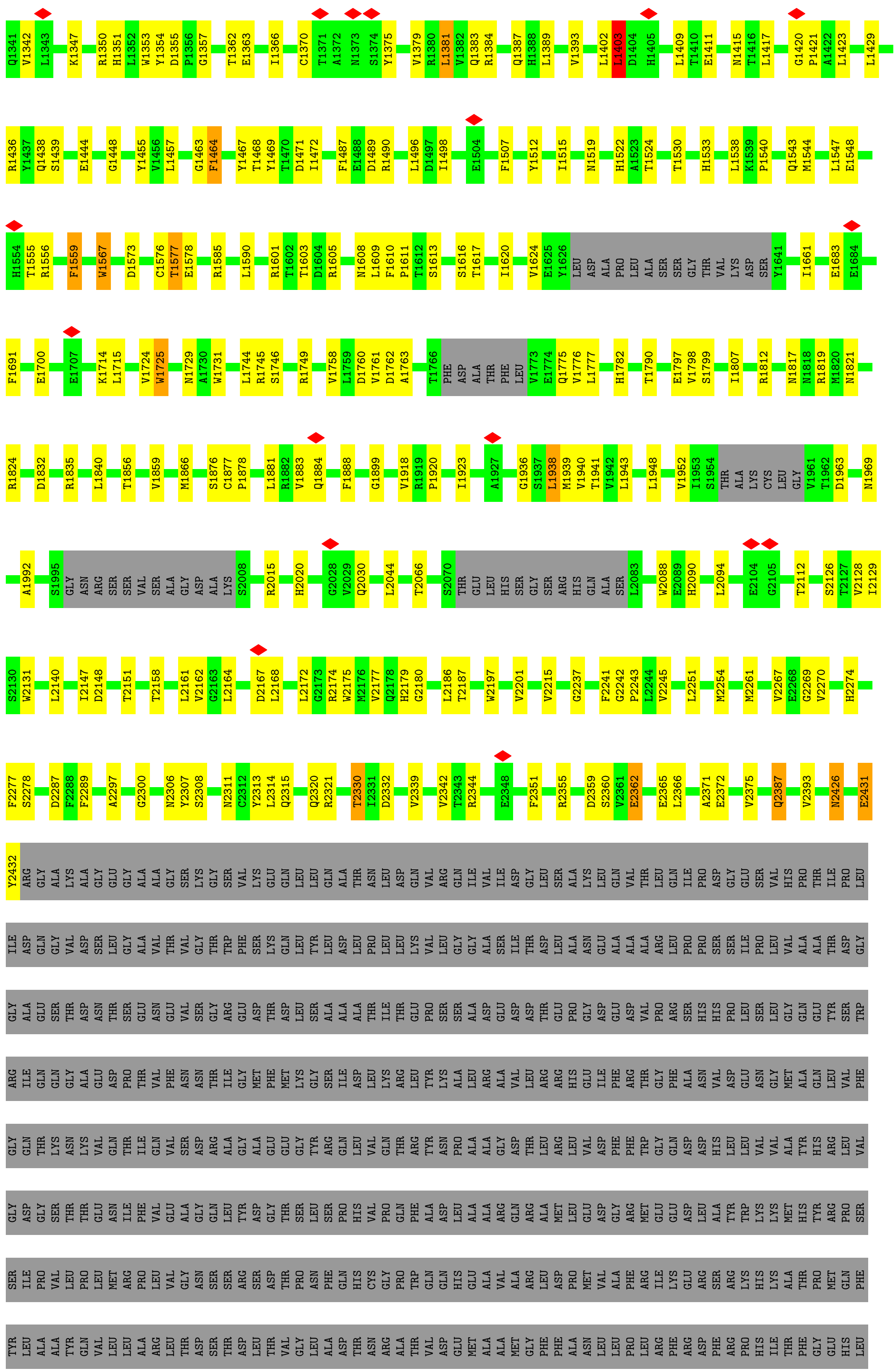


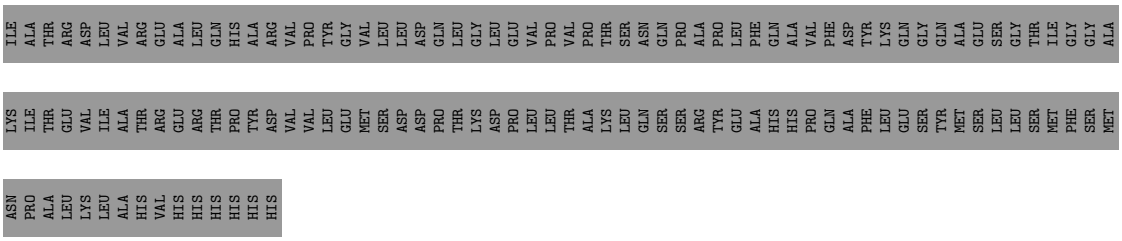


• Molecule 2: Lovastatin nonaketide synthase, polyketide synthase component

Chain A:

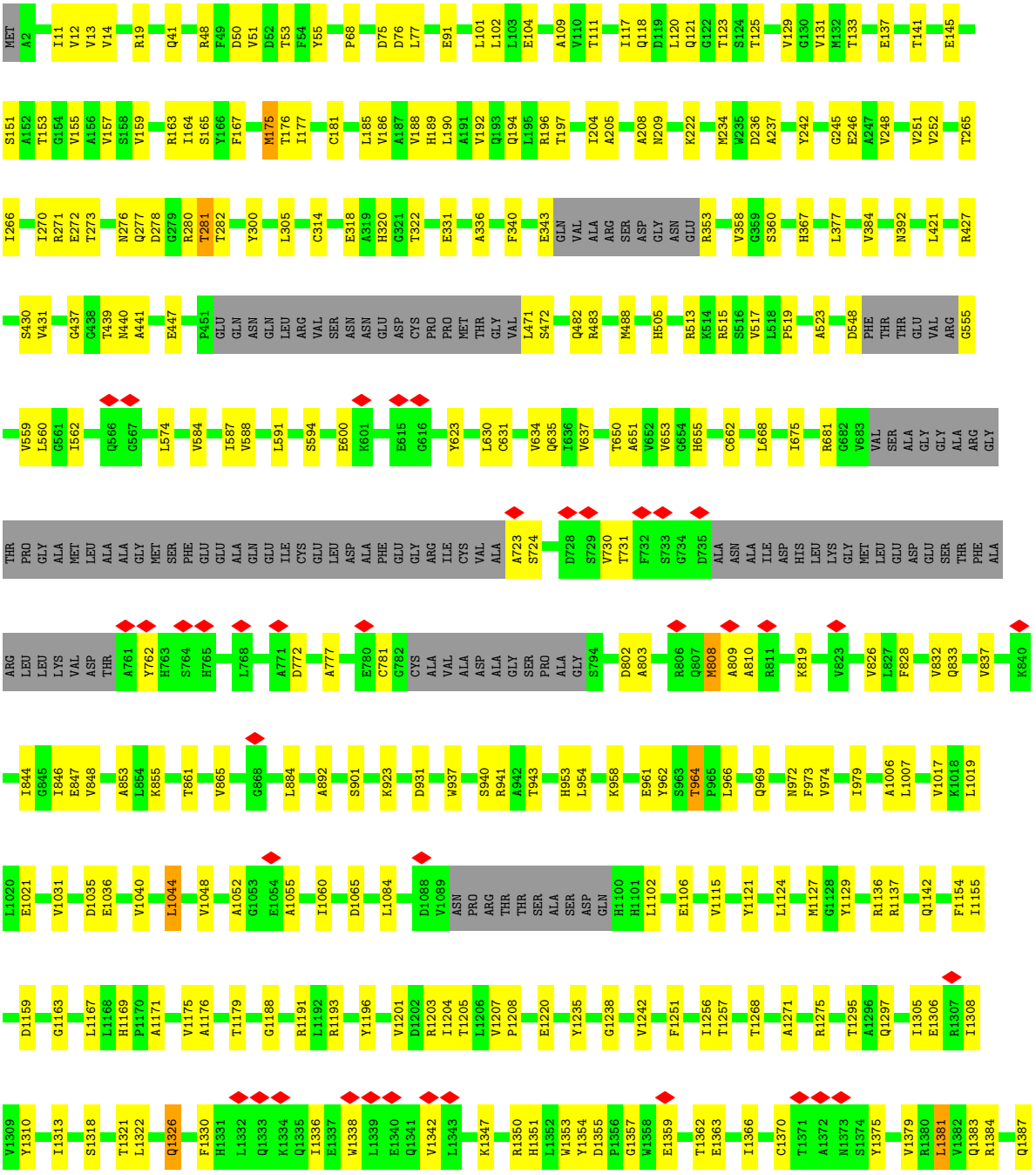


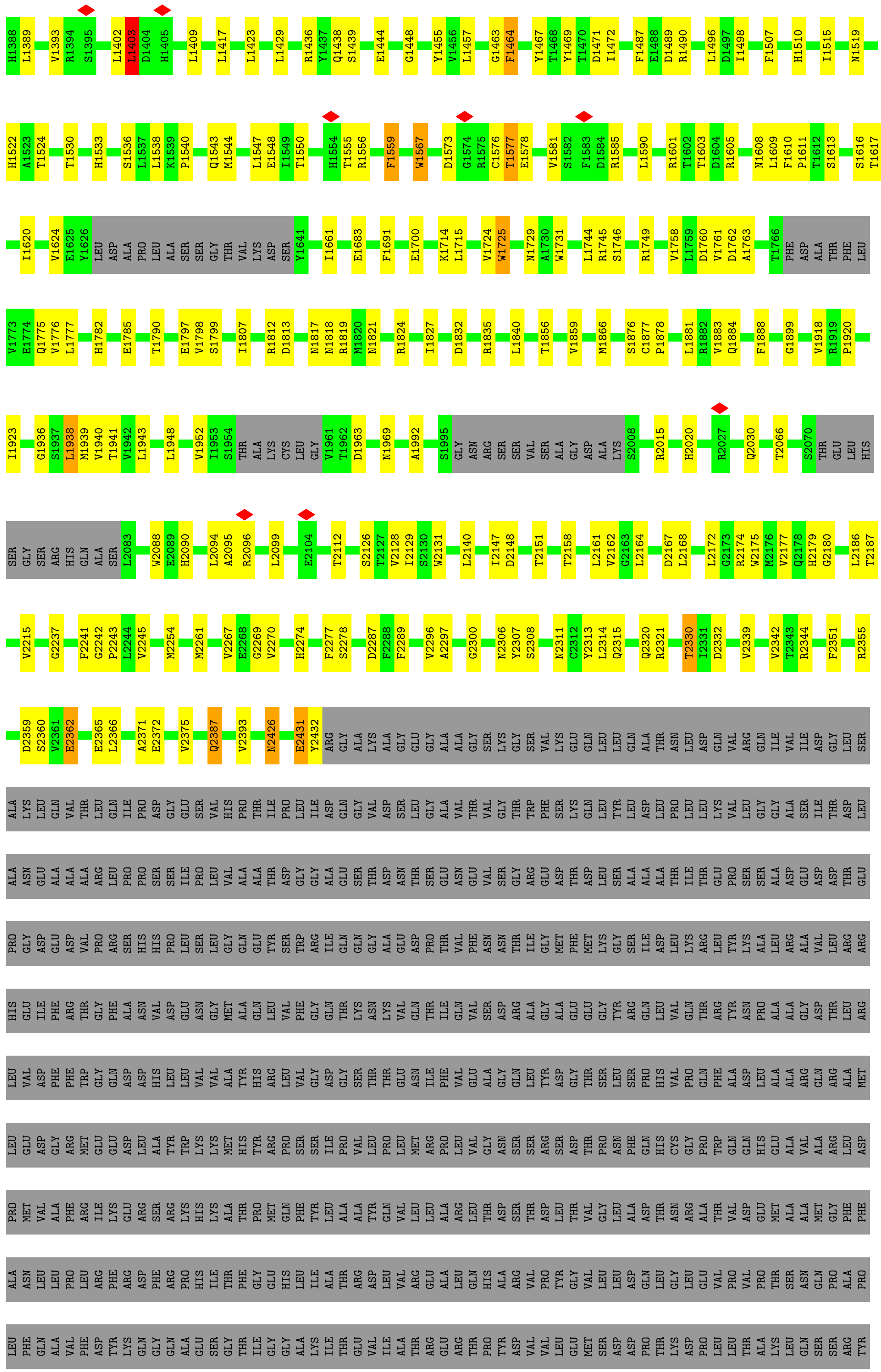

Q1341 V1342 L1343 K1347 R1350 H1351 L1352 W1353 Y1354 D1355 P1356 G1357 T1362 E1363 I1366 C1370 T1371 A1372 N1373 S1374 Y1375 V1379 R1380 L1381 V1382 Q1383 R1384 Q1387 H1388 L1389 V1393 L1402 L1403 D1404 H1405 L1409 T1410 E1411 N1415 T1416 L1417 G1420 P1421 A1422 L1423 L1429
R1436 Y1437 Q1438 S1439 E1444 G1448 Y1455 V1456 L1457 G1463 F1464 Y1467 T1468 Y1469 T1470 D1471 I1472 F1487 E1488 D1489 R1490 L1496 D1497 I1498 E1504 F1507 Y1512 I1515 N1519 H1522 A1523 T1524 T1530 H1533 L1538 K1539 P1540 Q1543 M1544 L1547 E1548
H1554 T1555 R1556 F1559 W1567 D1573 C1576 T1577 E1578 R1585 L1590 R1601 T1602 T1603 D1604 R1605 N1608 L1609 F1610 P1611 T1612 S1613 S1616 T1617 I1620 V1624 E1625 Y1626 LEU ASP ALA PRO LEU ALA SER SER GLY THR VAL LYS ASP SER Y1641 I1661 E1683 E1684
F1691 E1700 E1707 K1714 L1715 V1724 W1725 N1729 A1730 W1731 L1744 R1745 S1746 R1749 V1758 L1759 D1760 V1761 D1762 A1763 T1766 PHE ASP ALA THR PHE LEU V1773 E1774 Q1775 V1776 L1777 H1782 T1790 E1797 V1798 S1799 I1807 R1812 N1817 N1818 R1819 M1820 N1821
R1824 D1832 R1835 L1840 T1856 V1859 M1866 S1876 C1877 P1878 L1881 R1882 V1883 Q1884 F1888 G1899 V1918 R1919 P1920 I1923 A1927 G1936 S1937 L1938 M1939 V1940 T1941 V1942 L1943 L1948 V1952 I1953 S1954 THR ALA LYS CYS LEU GLY V1961 T1962 D1963 N1969
A1992 S1995 GLY ASN ARG SER SER VAL SER ALA GLY ASP ALA LYS S2008 R2015 H2020 G2028 V2029 Q2030 L2044 T2066 S2070 THR GLU LEU HIS SER GLY SER ARG HIS GLN ALA SER L2083 W2088 E2089 H2090 L2094 E2104 G2105 T2112 S2126 T2127 V2128 I2129
S2130 W2131 L2140 I2147 D2148 T2151 T2158 L2161 V2162 G2163 L2164 D2167 L2168 L2172 G2173 R2174 W2175 M2176 V2177 Q2178 H2179 G2180 L2186 T2187 W2197 V2201 V2215 G2237 F2241 G2242 P2243 L2244 V2245 L2251 M2254 M2261 V2267 E2268 G2269 V2270 H2274
F2277 S2278 D2287 F2288 F2289 A2297 G2300 N2306 Y2307 S2308 N2311 G2312 Y2313 L2314 Q2315 Q2320 R2321 T2330 I2331 D2332 V2339 V2342 T2343 R2344 E2348 F2351 R2355 D2359 S2360 V2361 E2362 E2365 L2366 A2371 E2372 V2375 Q2387 V2393 N2426 E2431
Y2432 ARG GLY ALA LYS ALA GLY GLU GLY ALA ALA GLY SER LYS GLY SER VAL LYS GLU GLN LEU LEU GLN ALA THR ASN LEU ASP GLN VAL ARG GLN ILE VAL ILE ASP GLY LEU SER ALA LYS LEU GLN VAL THR LEU GLN ILE PRO ASP GLY GLU SER VAL HIS PRO THR ILE PRO LEU
ILE ASP GLN GLY VAL ASP SER LEU GLY ALA VAL THR VAL GLY THR TRP PHE SER LYS GLN LEU TYR LEU ASP LEU PRO LEU LEU LYS VAL LEU GLY GLY ALA SER ILE THR ASP LEU ALA ASN GLU ALA ALA ALA ARG LEU PRO PRO SER SER ILE PRO LEU VAL ALA ALA THR ASP GLY
GLY ALA GLU SER THR ASP ASN THR SER GLU ASN GLU VAL SER GLY ARG GLU ASP THR ASP LEU SER ALA ALA ALA THR ILE THR GLU PRO SER SER ALA ASP GLU ASP ASP THR GLU PRO GLY ASP GLU ASP VAL PRO ARG SER HIS HIS PRO LEU SER LEU GLY GLN GLU TYR SER TRP
ARG ILE GLN GLN GLY ALA GLU ASP PRO THR VAL PHE ASN ASN THR ILE GLY MET PHE MET LYS GLY SER ILE ASP LEU LYS ARG LEU TYR LYS ALA LEU ARG ALA VAL LEU ARG ARG HIS GLU ILE PHE ARG THR GLY PHE ALA ASN VAL ASP GLU ASN GLY MET ALA GLN LEU VAL PHE
GLY GLN THR LYS ASN LYS VAL GLN THR ILE GLN VAL SER ASP ARG ALA GLY ALA GLU GLU GLY TYR ARG GLN LEU VAL GLN THR ARG TYR ASN PRO ALA ALA GLY ASP THR LEU ARG LEU VAL ASP PHE PHE TRP GLY GLN ASP ASP HIS LEU LEU VAL VAL ALA TYR HIS ARG LEU VAL
GLY ASP GLY SER THR THR GLU ASN ILE PHE VAL GLU ALA GLY GLN LEU TYR ASP GLY THR SER LEU SER PRO HIS VAL PRO GLN PHE ALA ASP LEU ALA ALA ARG GLN ARG ALA MET LEU GLU ASP GLY ARG MET GLU GLU ASP LEU ALA TYR TRP LYS LYS MET HIS TYR ARG PRO SER
SER ILE PRO VAL LEU PRO LEU MET ARG PRO LEU VAL GLY ASN SER SER ARG SER ASP THR PRO ASN PHE GLN HIS CYS GLY PRO TRP GLN GLN HIS GLU ALA VAL ALA ARG LEU ASP PRO MET VAL ALA PHE ARG ILE LYS GLU ARG SER ARG LYS HIS LYS ALA THR PRO MET GLN PHE
TYR LEU ALA ALA TYR GLN VAL LEU LEU ALA ARG LEU THR ASP SER THR ASP LEU THR VAL GLY LEU ALA ASP THR ASN ARG ALA THR VAL ASP GLU MET ALA ALA MET GLY PHE PHE ALA ASN LEU LEU PRO LEU ARG PHE ARG ASP PHE ARG PRO HIS ILE THR PHE GLY GLU HIS LEU



• Molecule 2: Lovastatin nonaketide synthase, polyketide synthase component

Chain B:

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H1522 A1523 T1524 T1530 H1533 S1536 L1537 L1538 K1539 P1540 Q1543 M1544 L1547 E1548 I1549 T1550 H1554 T1555 R1556 F1559 W1567 D1573 G1574 R1575 C1576 T1577 E1578 V1581 S1582 F1583 D1584 R1585 L1590 R1601 T1602 T1603 D1604 R1605 N1608 L1609 F1610 P1611 T1612 S1613 S1616 T1617
I1620 V1624 E1625 Y1626 LEU ASP ALA PRO LEU ALA SER SER GLY THR VAL LYS ASP SER Y1641 I1661 E1683 F1691 E1700 K1714 L1715 V1724 W1725 N1729 A1730 W1731 L1744 R1745 S1746 R1749 V1758 L1759 D1760 V1761 D1762 A1763 T1766 PHE ASP ALA THR PHE LEU
V1773 E1774 Q1775 V1776 L1777 H1782 E1785 T1790 E1797 V1798 S1799 I1807 R1812 D1813 N1817 N1818 R1819 M1820 N1821 R1824 I1827 D1832 R1835 L1840 T1856 V1859 M1866 S1876 C1877 P1878 L1881 R1882 V1883 Q1884 F1888 G1899 V1918 R1919 P1920
I1923 G1936 S1937 L1938 M1939 V1940 T1941 V1942 L1943 L1948 V1952 I1953 S1954 THR ALA LYS CYS LEU GLY V1961 T1962 D1963 N1969 A1992 S1995 GLY ASN ARG SER SER VAL SER ALA GLY ASP ALA LYS S2008 R2015 H2020 R2027 Q2030 T2066 S2070 THR GLU LEU HIS
SER GLY SER ARG HIS GLN ALA SER L2083 W2088 E2089 H2090 L2094 A2095 R2096 L2099 E2104 T2112 S2126 T2127 V2128 I2129 S2130 W2131 L2140 I2147 D2148 T2151 T2158 L2161 V2162 G2163 L2164 D2167 L2168 L2172 G2173 R2174 W2175 M2176 V2177 Q2178 H2179 G2180 L2186 T2187
V2215 G2237 F2241 G2242 P2243 L2244 V2245 M2254 M2261 V2267 E2268 G2269 V2270 H2274 F2277 S2278 D2287 F2288 F2289 V2296 A2297 G2300 N2306 Y2307 S2308 N2311 C2312 Y2313 L2314 Q2315 Q2320 R2321 T2330 I2331 D2332 V2339 V2342 T2343 R2344 F2351 R2355
D2359 S2360 V2361 E2362 E2365 L2366 A2371 E2372 V2375 Q2387 V2393 N2426 E2431 Y2432 ARG GLY ALA LYS ALA GLY GLU GLY ALA ALA GLY SER LYS GLY SER VAL LYS GLU GLN LEU LEU GLN ALA THR ASN LEU ASP GLN VAL ARG GLN ILE VAL ILE ASP GLY LEU SER
ALA LYS LEU GLN VAL THR LEU GLN ILE PRO ASP GLY GLU SER VAL HIS PRO THR ILE PRO LEU ILE ASP GLN GLY VAL ASP SER LEU GLY ALA VAL THR VAL GLY THR TRP PHE SER LYS GLN LEU TYR LEU ASP LEU PRO LEU LEU LYS VAL LEU GLY GLY ALA SER ILE THR ASP LEU
ALA ASN GLU ALA ALA ALA ARG LEU PRO PRO SER SER ILE PRO LEU VAL ALA ALA THR ASP GLY GLY ALA GLU SER THR ASP ASN THR SER GLU ASN GLU VAL SER GLY ARG GLU ASP THR ASP LEU SER ALA ALA ALA THR ILE THR GLU PRO SER SER ALA ASP GLU ASP ASP THR GLU
PRO GLY ASP GLU ASP VAL PRO ARG SER HIS HIS PRO LEU SER LEU GLY GLN GLU TYR SER TRP ARG ILE GLN GLN GLY ALA GLU ASP PRO THR VAL PHE ASN ASN THR ILE GLY MET PHE MET LYS GLY SER ILE ASP LEU LYS ARG LEU TYR LYS ALA LEU ARG ALA ALA VAL LEU ARG ARG
HIS GLU ILE PHE ARG THR GLY PHE ALA ASN VAL ASP GLU ASN GLY MET ALA GLN LEU VAL PHE GLY GLN THR LYS ASN LYS VAL GLN THR ILE GLN VAL SER ASP ARG ALA GLY ALA GLU GLU GLY TYR ARG GLN LEU VAL GLN THR ARG TYR ASN PRO ALA ALA GLY ASP THR LEU ARG
LEU VAL ASP PHE PHE TRP GLY GLN ASP ASP HIS LEU LEU VAL VAL ALA TYR HIS ARG LEU VAL GLY ASP GLY SER THR THR GLU ASN ILE PHE VAL GLU ALA GLY GLN LEU TYR ASP GLY THR SER LEU SER PRO HIS VAL PRO GLN PHE ALA ASP LEU ALA ALA ARG GLN ARG ALA MET
LEU GLU ASP GLY ARG MET GLU GLU ASP LEU ALA TYR TRP LYS LYS MET HIS TYR ARG PRO SER SER ILE PRO VAL LEU PRO LEU MET ARG PRO LEU VAL GLY ASN SER SER ARG SER ASP THR PRO ASN PHE GLN HIS CYS GLY PRO TRP GLN GLN HIS GLU ALA VAL ALA ARG LEU ASP
PRO MET VAL ALA PHE ARG ILE LYS GLU ARG SER ARG LYS HIS LYS ALA THR PRO MET GLN PHE TYR LEU ALA ALA TYR GLN VAL LEU LEU ALA ARG LEU THR ASP SER THR ASP LEU THR VAL GLY LEU ALA ASP THR ASN ARG ALA THR VAL ASP GLU MET ALA ALA MET GLY PHE PHE
ALA ASN LEU LEU PRO LEU ARG PHE ARG ASP PHE ARG PRO HIS ILE THR PHE GLY GLU HIS LEU ILE ALA THR ARG ASP LEU VAL ARG GLU ALA LEU GLN HIS ALA ARG VAL PRO TYR GLY VAL LEU LEU ASP GLN LEU GLY LEU GLU VAL PRO VAL PRO THR SER ASN GLN PRO ALA PRO
LEU PHE GLN ALA VAL PHE ASP TYR LYS GLN GLY GLN ALA GLU SER GLY THR ILE GLY GLY ALA LYS ILE THR GLU VAL ILE ALA THR ARG GLU ARG THR PRO TYR ASP VAL VAL LEU GLU MET SER ASP ASP PRO THR LYS ASP PRO LEU LEU THR ALA LYS LEU GLN SER SER ARG TYR

GLU
ALA
HIS
HIS
PRO
GLN
ALA
PHE
LEU
GLU
SER
TYR
MET
SER
LEU
LEU
SER
MET
PHE
SER
MET
ASN
PRO
ALA
LEU
LYS
LEU
ALA
HIS
VAL
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83573	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 ($e^-/Å^2$)	60.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0082	Depositor
Map size (Å)	350.0, 350.0, 350.0	wwPDB
Map dimensions	350, 350, 350	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

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

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	C	0.77	0/2815	0.76	2/3842 (0.1%)
1	D	0.77	0/2815	0.76	2/3842 (0.1%)
2	A	0.24	0/18071	0.49	2/24587 (0.0%)
2	B	0.24	0/18071	0.49	2/24587 (0.0%)
All	All	0.36	0/41772	0.54	8/56858 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	LEU	CB-CG-CD1	5.85	120.94	111.00
2	A	1403	LEU	CA-CB-CG	5.84	128.74	115.30
1	D	147	LEU	CB-CG-CD1	5.83	120.91	111.00
2	B	1403	LEU	CA-CB-CG	5.83	128.70	115.30
2	A	1899	GLY	C-N-CA	5.50	135.45	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2742	0	2694	51	0
1	D	2742	0	2694	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	17652	17336	17276	304	0
2	B	17652	17336	17276	305	0
3	A	48	25	25	0	0
3	B	48	25	25	0	0
All	All	40884	34722	39990	692	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 692 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:D:361:GLU:O	1:D:361:GLU:HG2	1.71	0.90
1:C:361:GLU:O	1:C:361:GLU:HG2	1.71	0.89
1:C:294:ALA:H	1:C:295:PRO:CD	1.89	0.85
2:A:2362:GLU:OE1	2:A:2362:GLU:N	2.10	0.84
1:D:294:ALA:H	1:D:295:PRO:CD	1.89	0.84

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	C	353/371 (95%)	340 (96%)	12 (3%)	1 (0%)	41 75
1	D	353/371 (95%)	340 (96%)	12 (3%)	1 (0%)	41 75
2	A	2236/3046 (73%)	2147 (96%)	88 (4%)	1 (0%)	100 100
2	B	2236/3046 (73%)	2146 (96%)	89 (4%)	1 (0%)	100 100
All	All	5178/6834 (76%)	4973 (96%)	201 (4%)	4 (0%)	54 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	ALA
1	D	294	ALA
2	A	1577	THR
2	B	1577	THR

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	C	292/303 (96%)	276 (94%)	16 (6%)	21	57
1	D	292/303 (96%)	276 (94%)	16 (6%)	21	57
2	A	1904/2547 (75%)	1854 (97%)	50 (3%)	46	74
2	B	1904/2547 (75%)	1854 (97%)	50 (3%)	46	74
All	All	4392/5700 (77%)	4260 (97%)	132 (3%)	44	71

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1715	LEU
2	B	1938	LEU
2	B	2426	ASN
2	A	964	THR
2	A	937	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	946	HIS
2	B	2387	GLN
2	A	2387	GLN
2	B	635	GLN
1	D	18	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)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	NAP	A	3500	-	45,52,52	2.65	16 (35%)	56,80,80	1.51	9 (16%)
3	NAP	B	3500	-	45,52,52	2.65	16 (35%)	56,80,80	1.51	9 (16%)

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
3	NAP	A	3500	-	-	12/31/67/67	0/5/5/5
3	NAP	B	3500	-	-	12/31/67/67	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500	NAP	O4B-C1B	8.71	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3500	NAP	O4B-C1B	8.70	1.53	1.41
3	A	3500	NAP	C7N-N7N	6.52	1.45	1.33
3	B	3500	NAP	C7N-N7N	6.50	1.45	1.33
3	A	3500	NAP	C2N-N1N	6.24	1.42	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3500	NAP	C6N-N1N-C2N	-5.68	116.79	121.97
3	B	3500	NAP	C6N-N1N-C2N	-5.57	116.89	121.97
3	B	3500	NAP	C3D-C2D-C1D	3.96	106.94	100.98
3	A	3500	NAP	C3D-C2D-C1D	3.93	106.90	100.98
3	A	3500	NAP	PN-O3-PA	-3.06	122.32	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

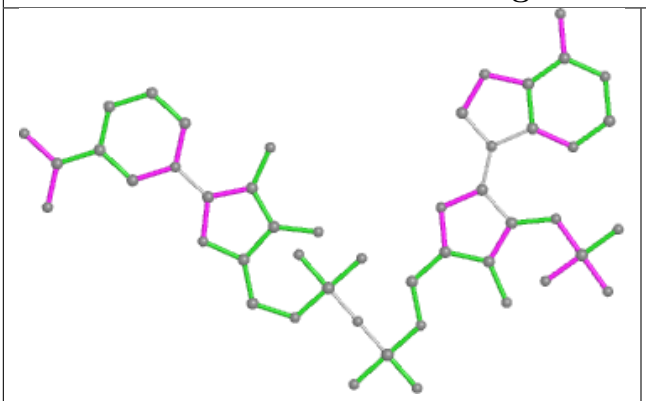
Mol	Chain	Res	Type	Atoms
3	A	3500	NAP	C5D-O5D-PN-O3
3	A	3500	NAP	C5D-O5D-PN-O2N
3	B	3500	NAP	C5D-O5D-PN-O3
3	B	3500	NAP	C5D-O5D-PN-O2N
3	A	3500	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

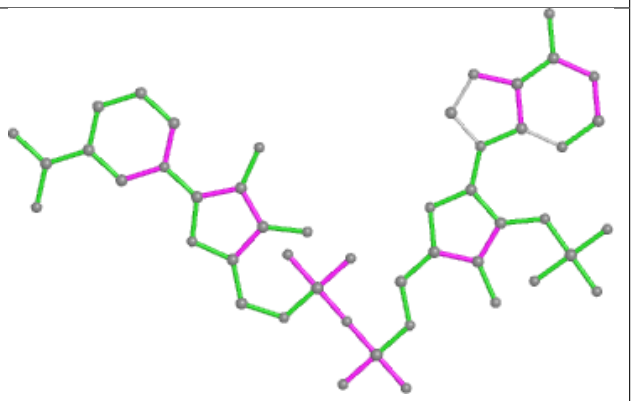
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

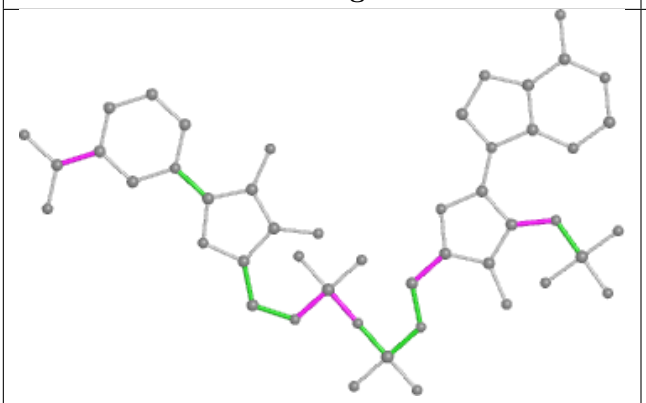
Ligand NAP A 3500



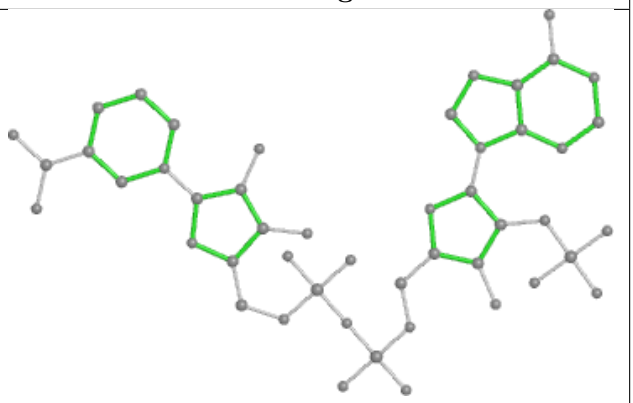
Bond lengths



Bond angles

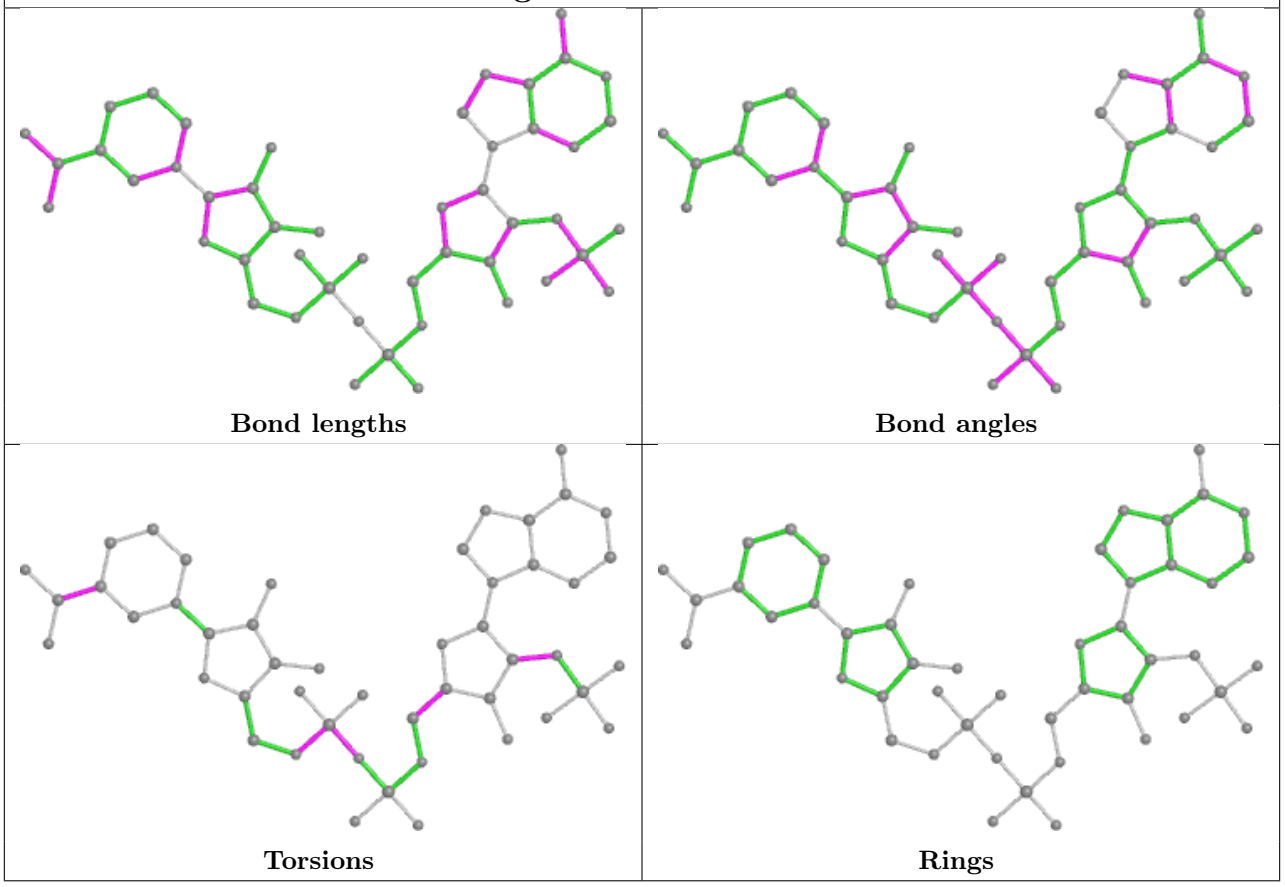


Torsions



Rings

Ligand NAP B 3500



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.

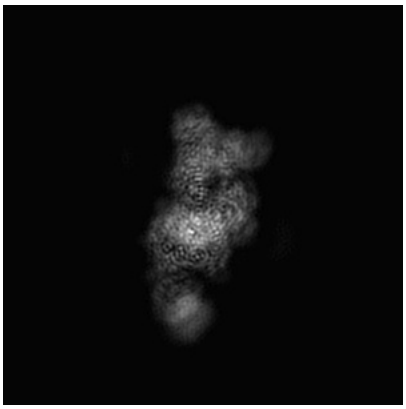
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30435. These allow visual inspection of the internal detail of the map and identification of artifacts.

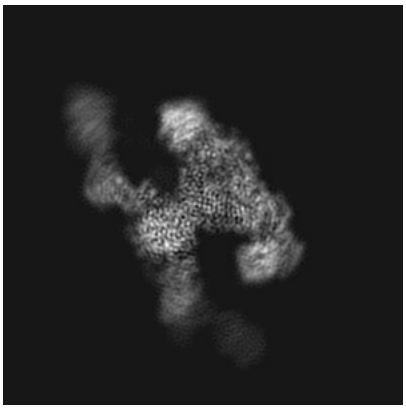
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

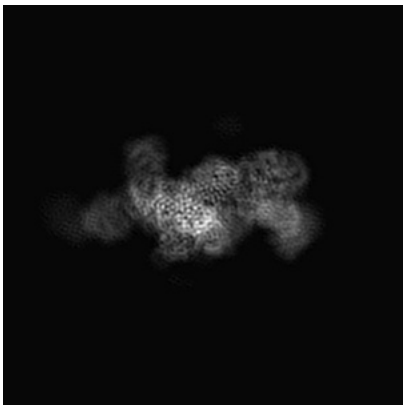
6.1.1 Primary map



X

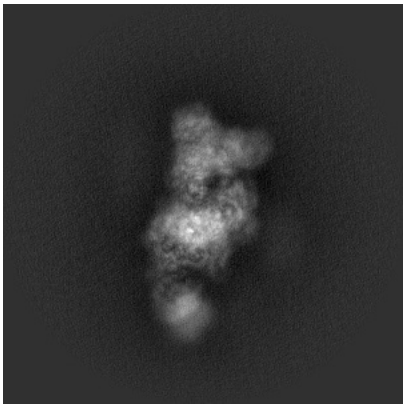


Y

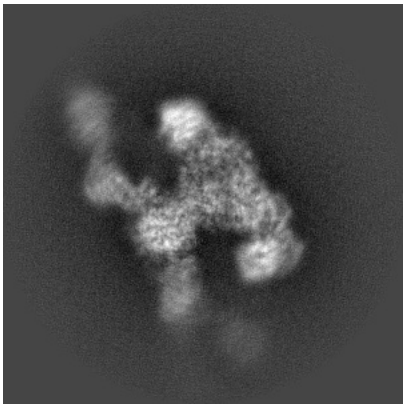


Z

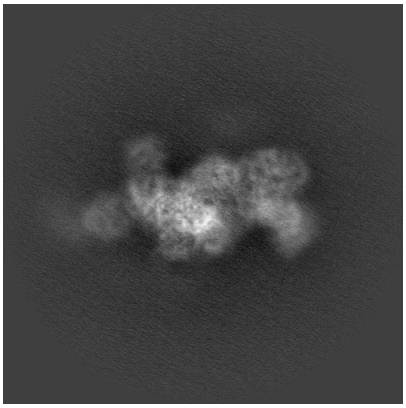
6.1.2 Raw map



X



Y



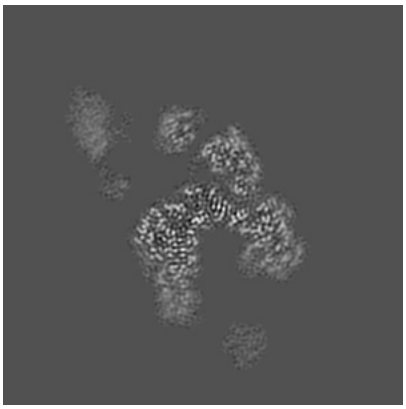
Z

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

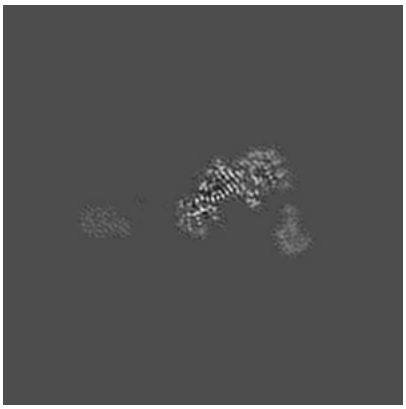
6.2 Central slices (i)

6.2.1 Primary map

X Index: 175

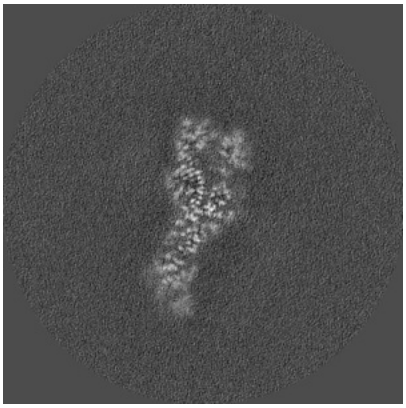


Y Index: 175

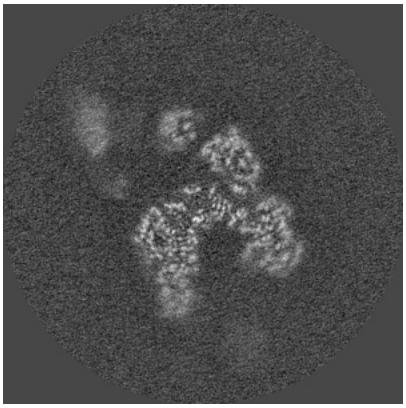


Z Index: 175

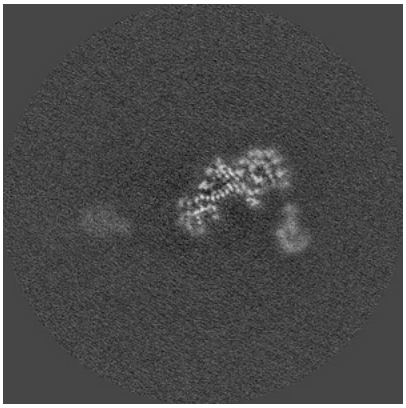
6.2.2 Raw map



X Index: 175



Y Index: 175

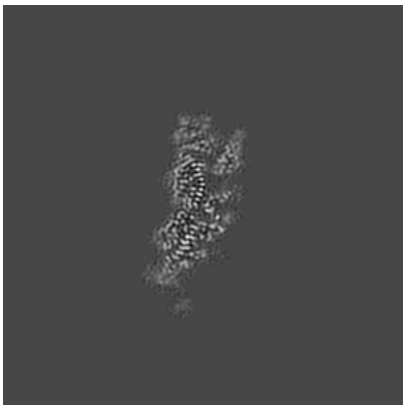


Z Index: 175

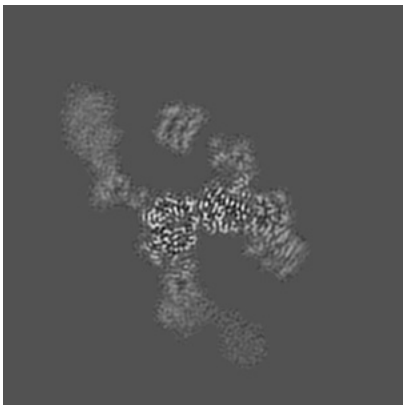
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

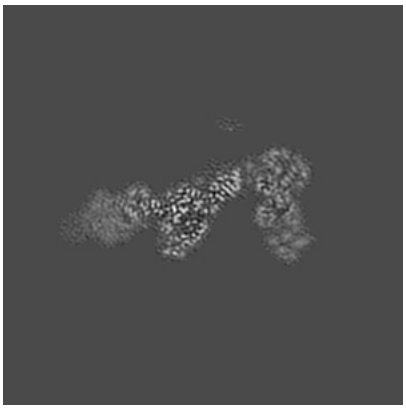
6.3.1 Primary map



X Index: 170

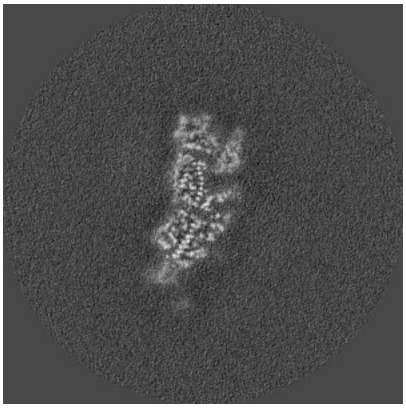


Y Index: 165

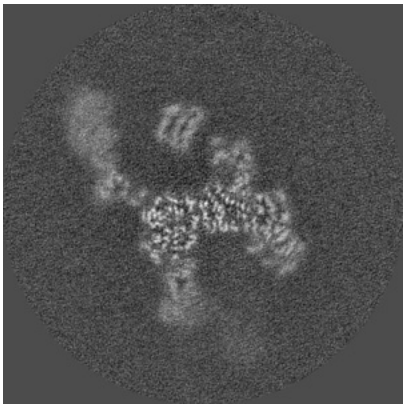


Z Index: 158

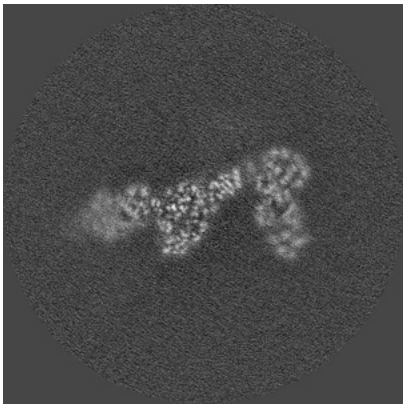
6.3.2 Raw map



X Index: 169



Y Index: 165

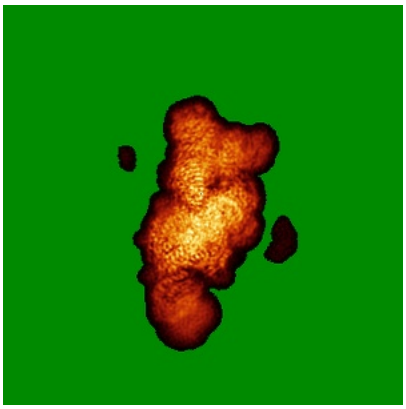


Z Index: 157

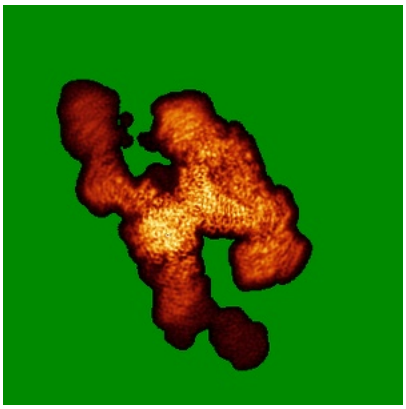
The images above show the largest variance slices of the map in three orthogonal directions.

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

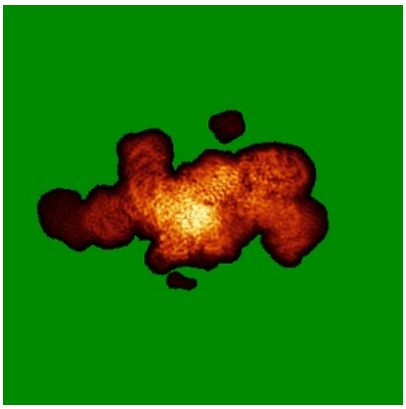
6.4.1 Primary map



X

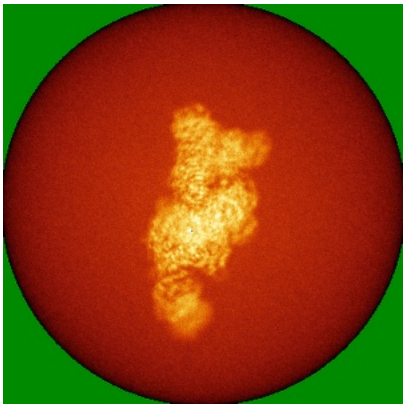


Y

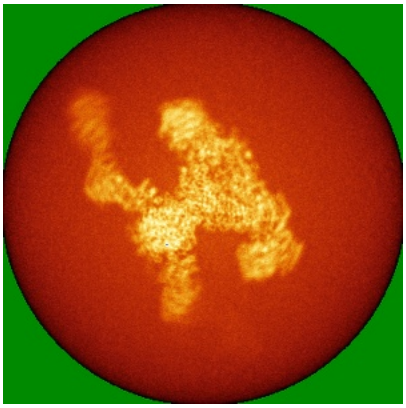


Z

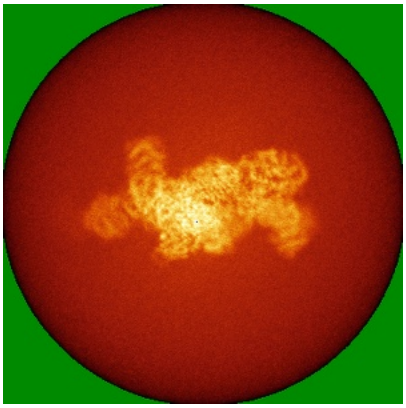
6.4.2 Raw map



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.

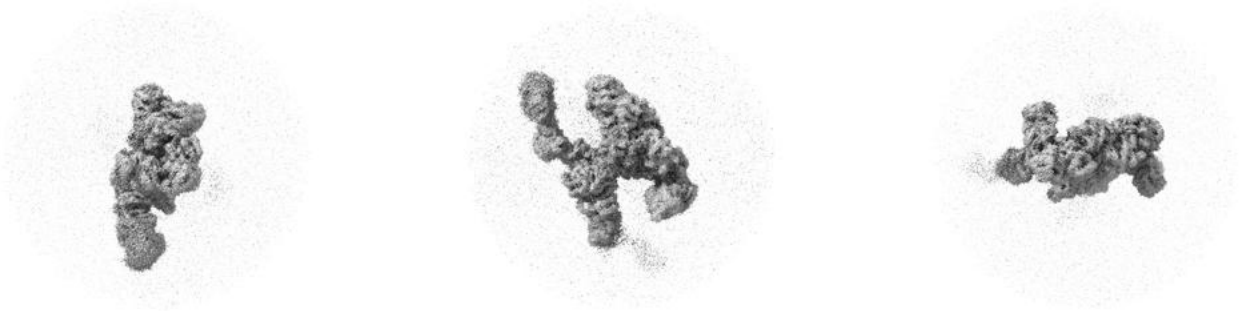
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0082. 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.

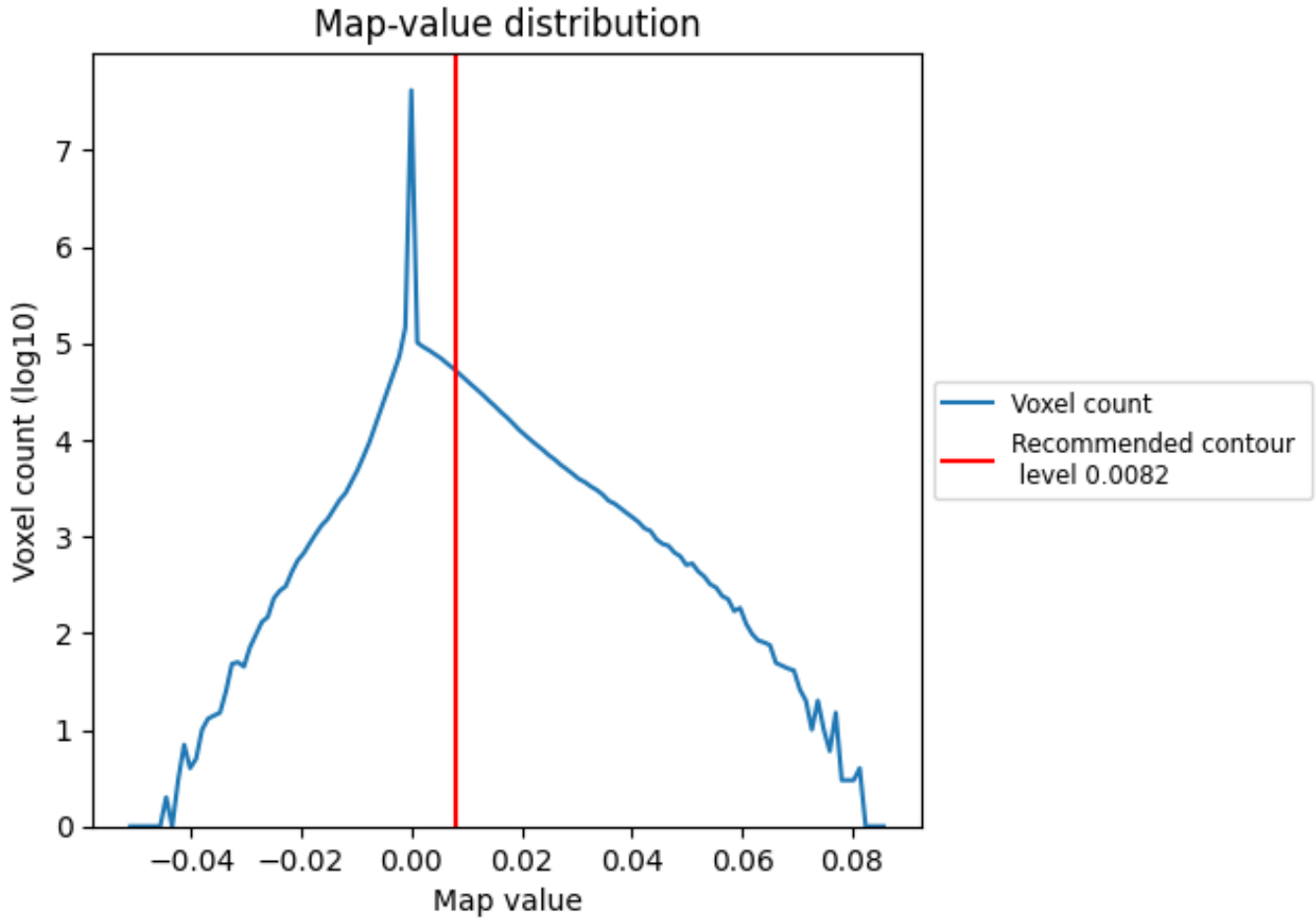
6.6 Mask visualisation (i)

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

7 Map analysis

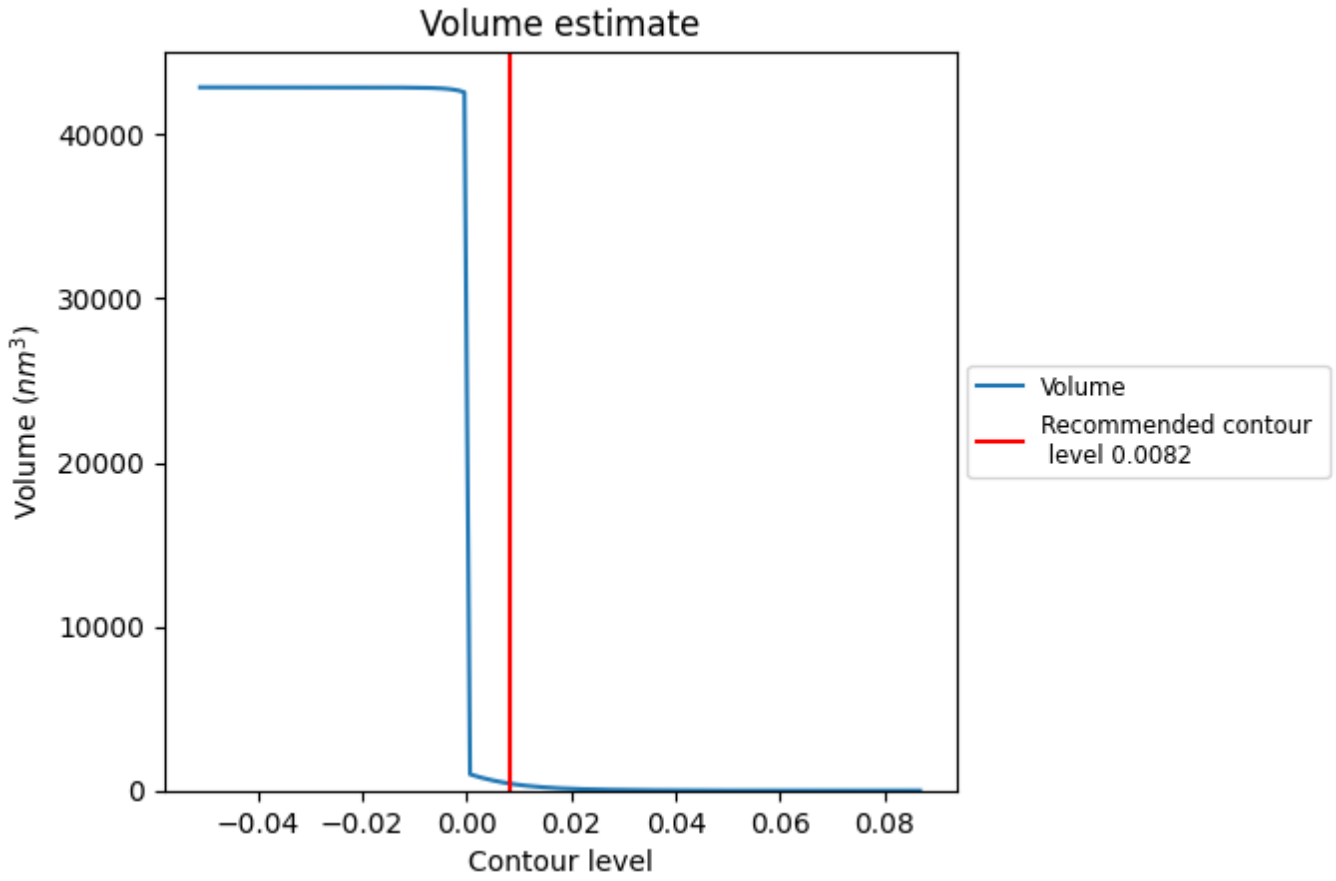
This section contains the results of statistical analysis of the map.

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.

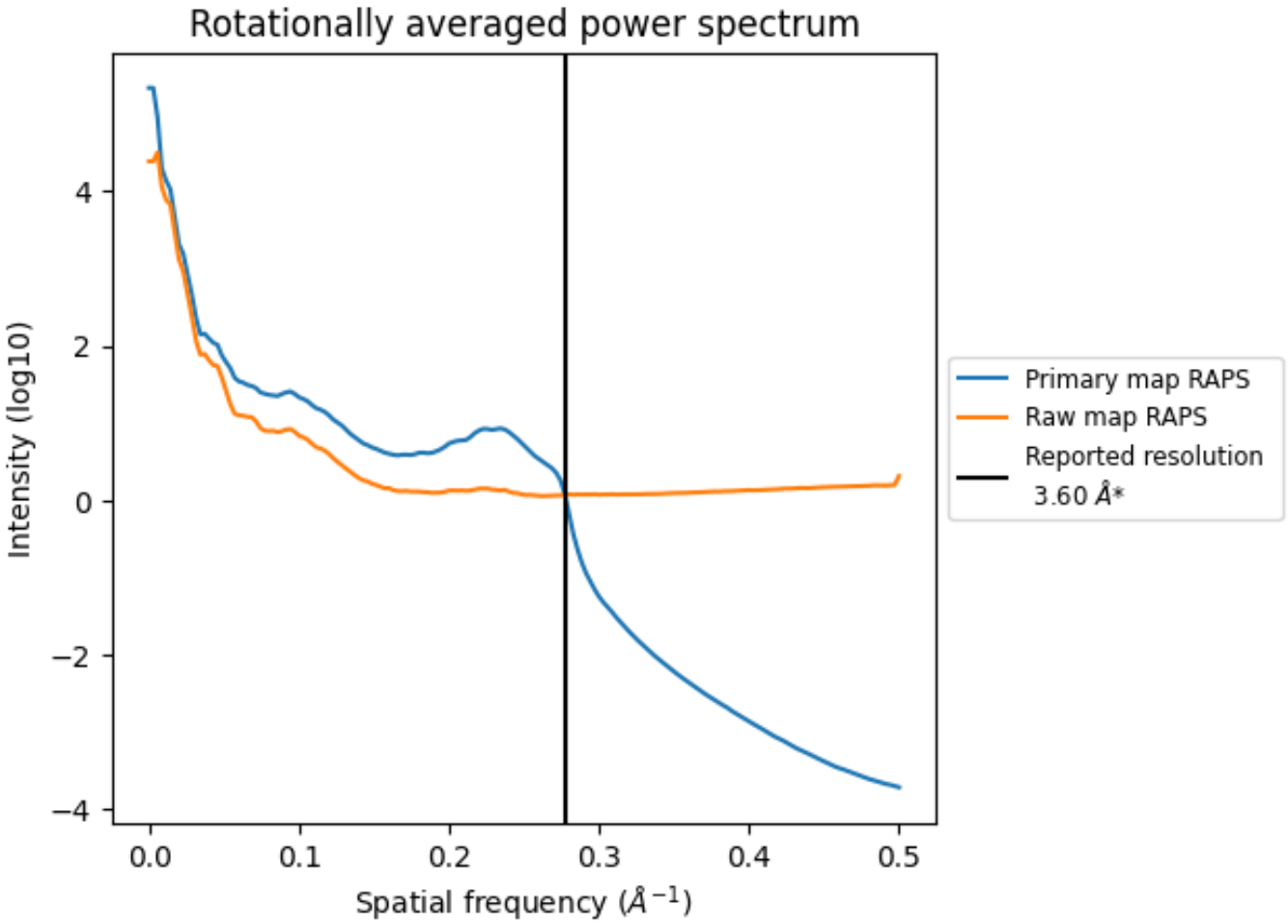
7.2 Volume estimate (i)



The volume at the recommended contour level is 429 nm^3; this corresponds to an approximate mass of 387 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)

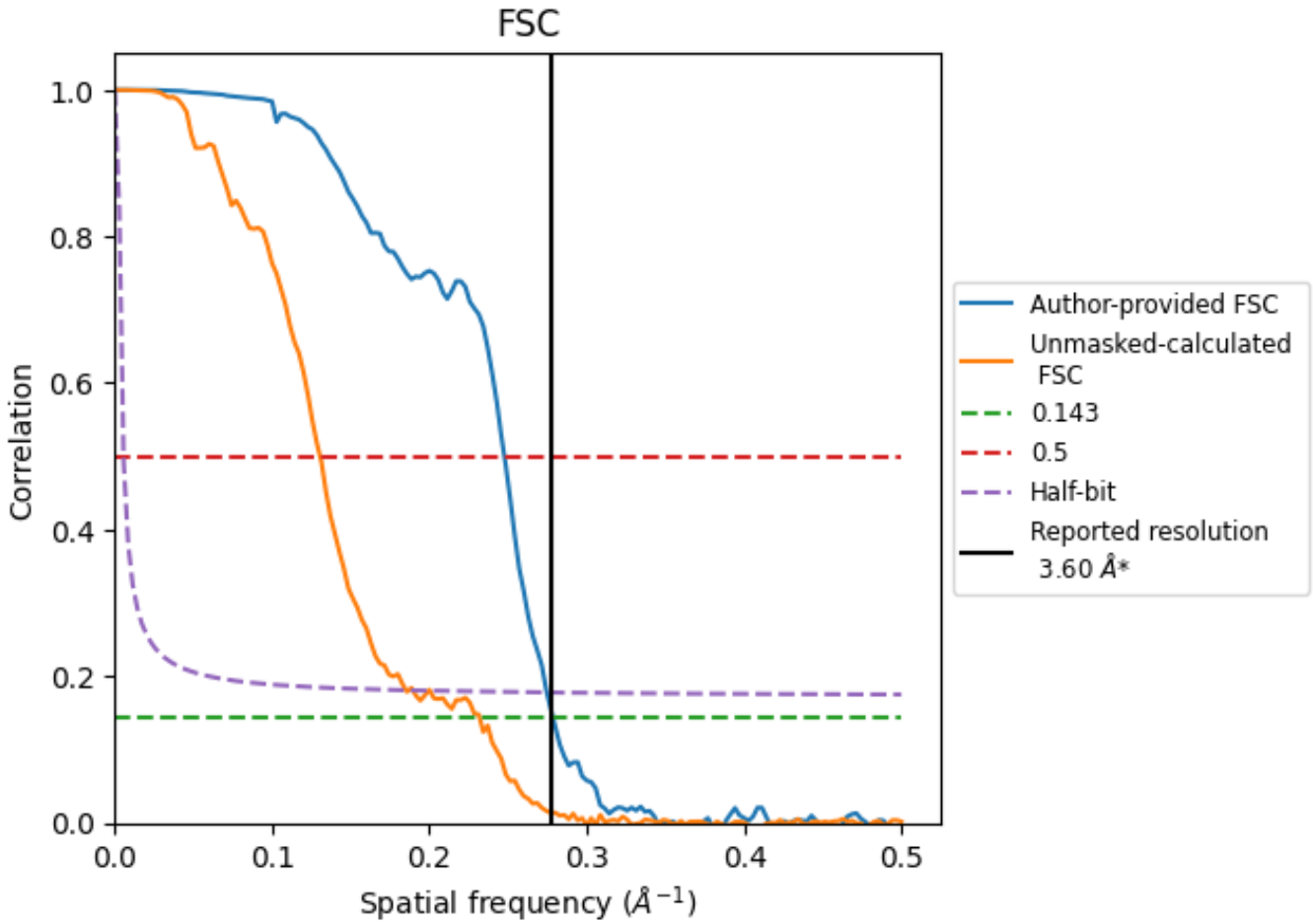


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

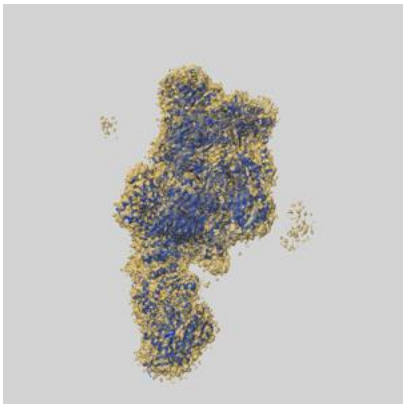
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.04	3.64
Unmasked-calculated*	4.31	7.66	5.40

*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 4.31 differs from the reported value 3.6 by more than 10 %

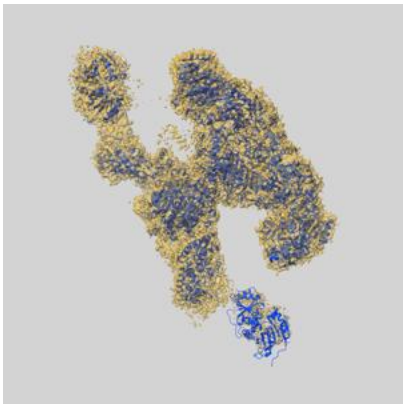
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30435 and PDB model 7CPY. Per-residue inclusion information can be found in section 3 on page 6.

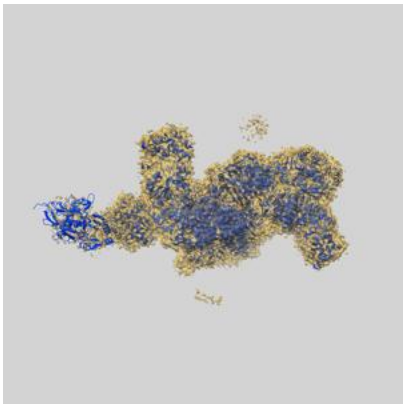
9.1 Map-model overlay



X



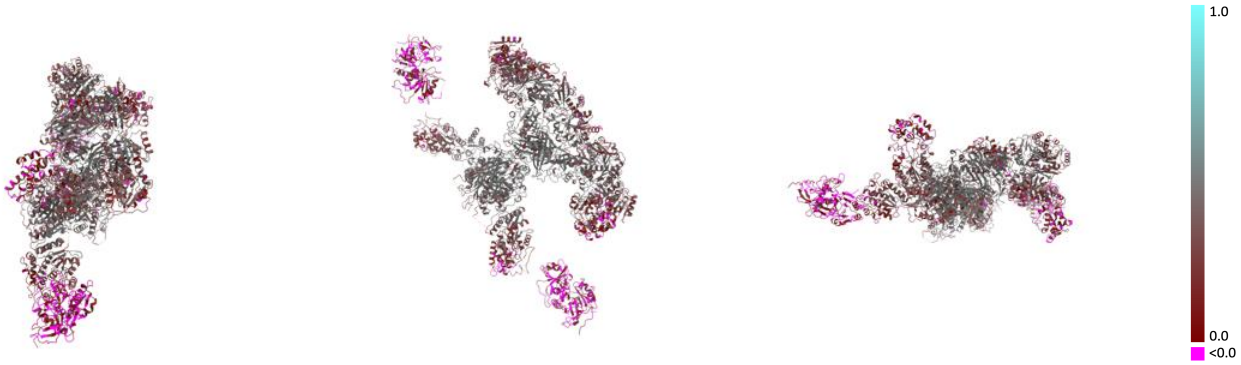
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0082 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.

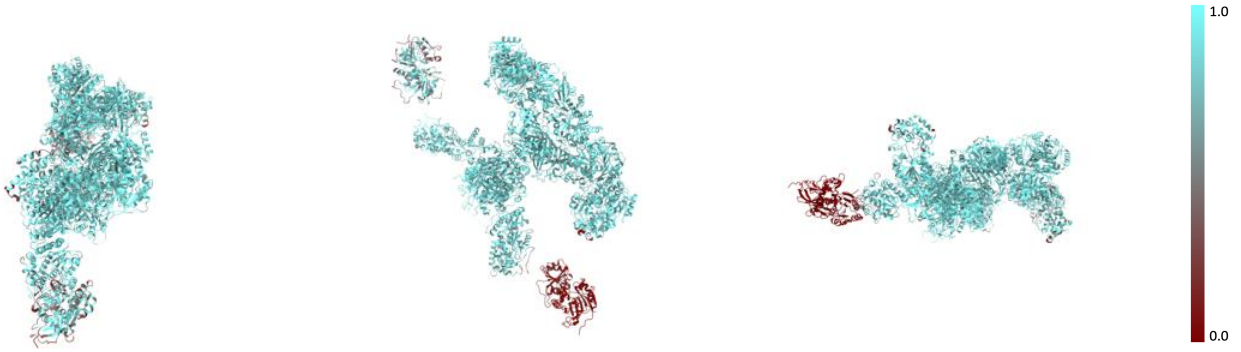
9.2 Q-score mapped to coordinate model



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.

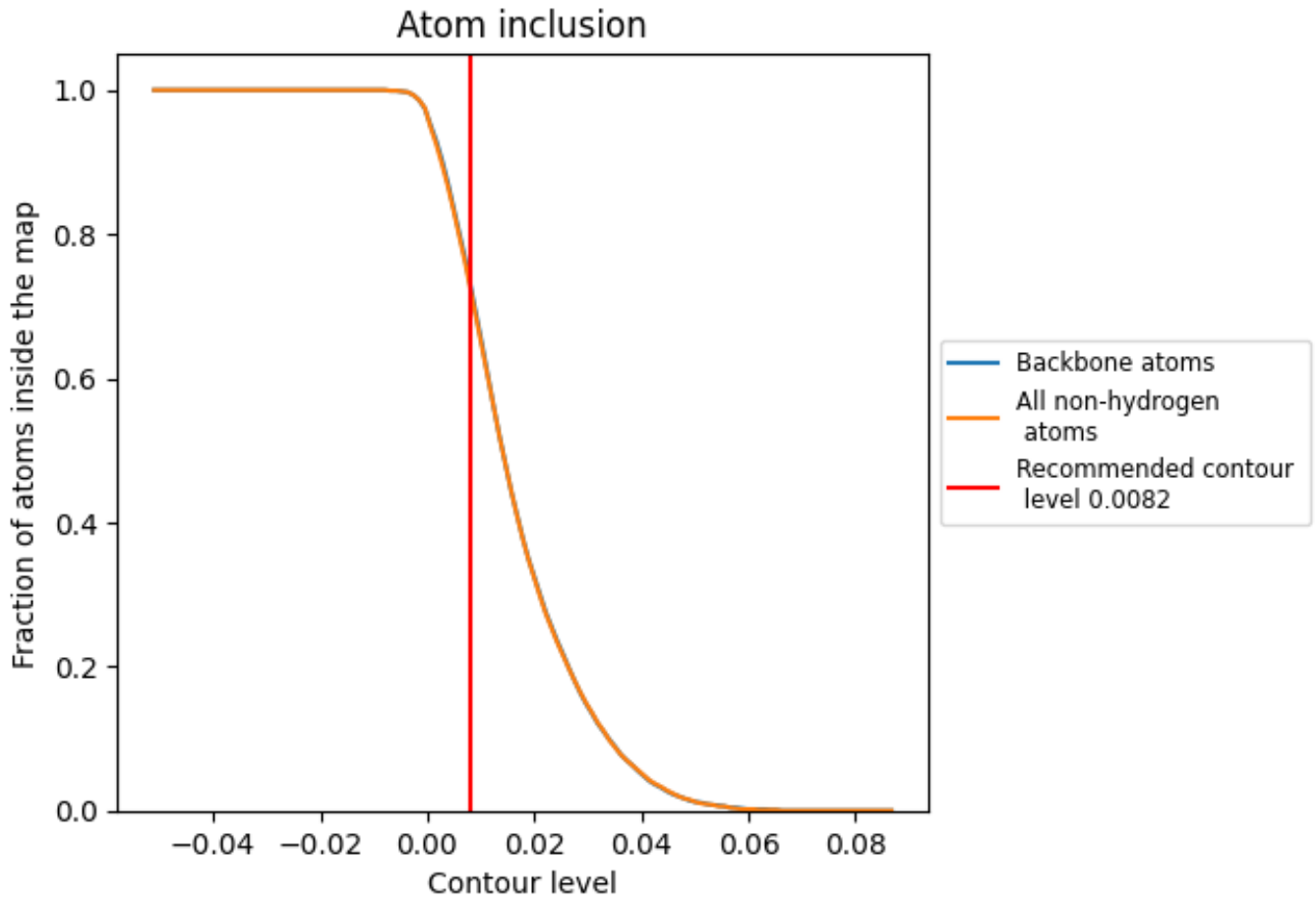
9.3 Atom inclusion mapped to coordinate model



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 (0.0082).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.3060
A	0.8570	0.3600
B	0.8420	0.3390
C	0.6200	0.0380
D	0.0300	0.0070