Full wwPDB EM Validation Report ⓘ

Oct 28, 2026 – 12:21 AM JST

PDB ID	:	27DN / pdb_000027dn
EMDB ID	:	EMD-81083
Title	:	Cryo-EM Structure of Hybrid NRPS-PKS Enzyme CorA from the myxobacterium Corallococcus exiguus
Authors	:	Qingyu, Y.; Hang, Z.; Wei, Z.
Deposited on	:	2026-05-27
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

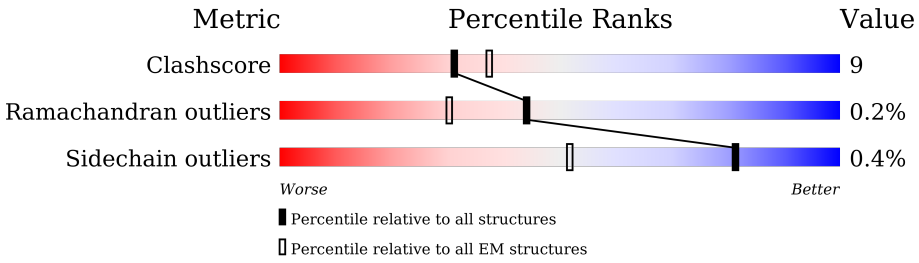
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

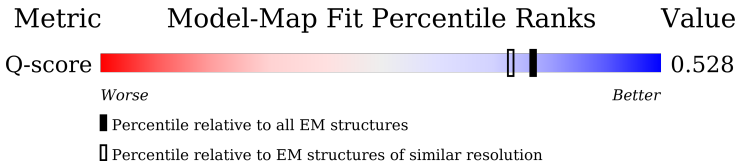
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2867	24% 6% 70%
1	B	2867	24% 6% 70%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13082 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 Linear gramicidin synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	873	Total	C	N	O	S	0	0
			6541	4115	1184	1224	18		
1	A	873	Total	C	N	O	S	0	0
			6541	4115	1184	1224	18		

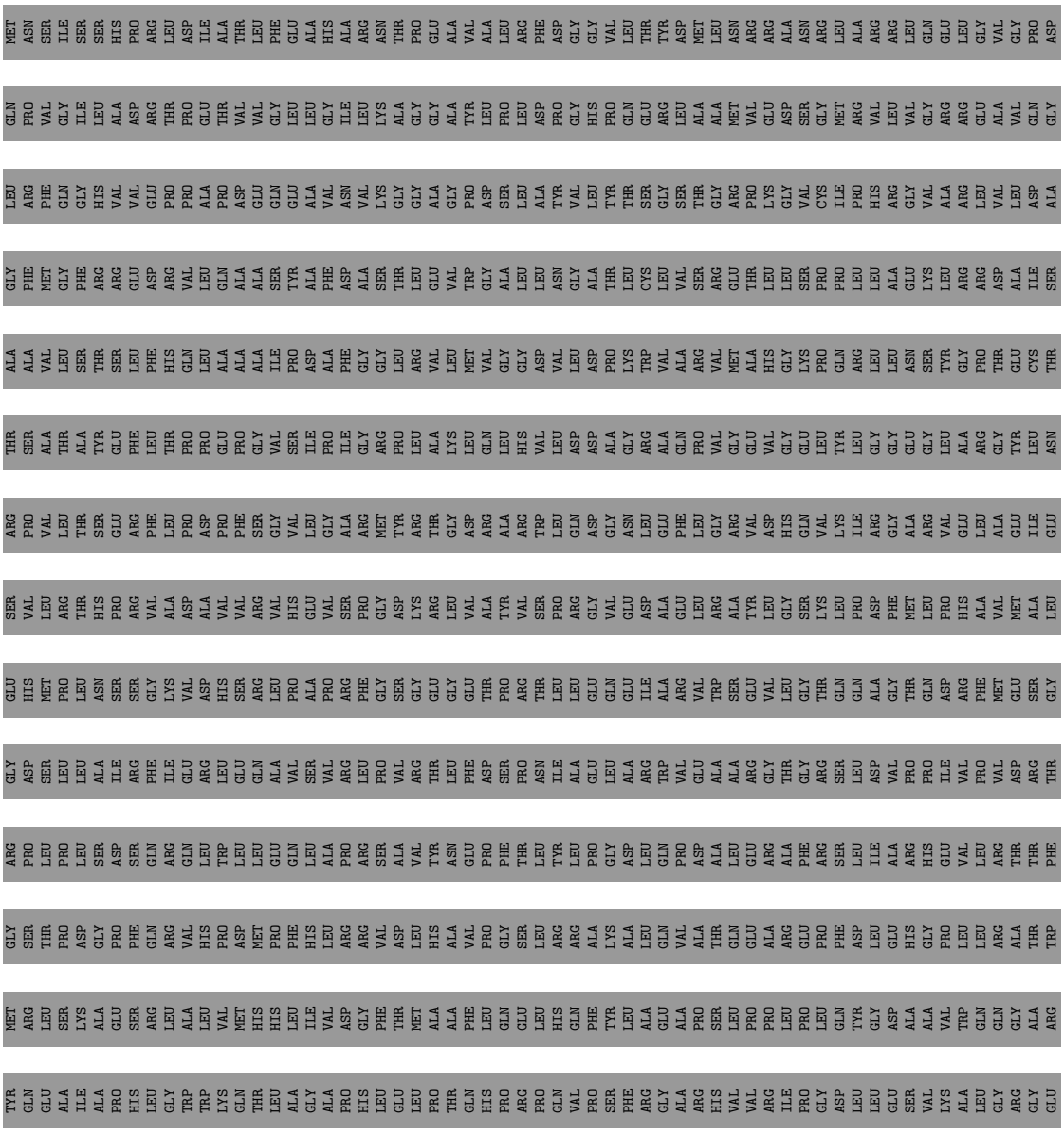
3 Residue-property plots (i)

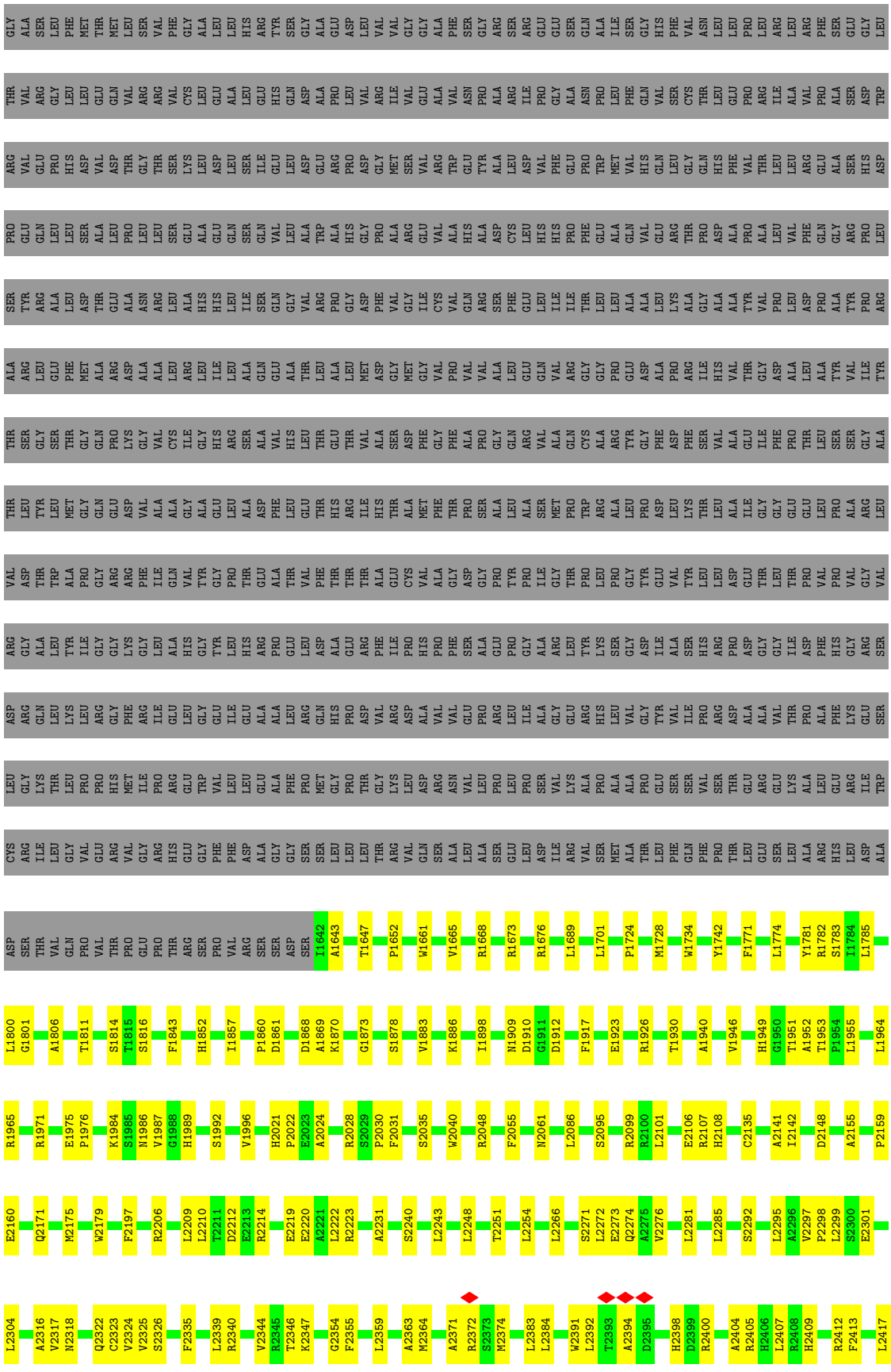
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

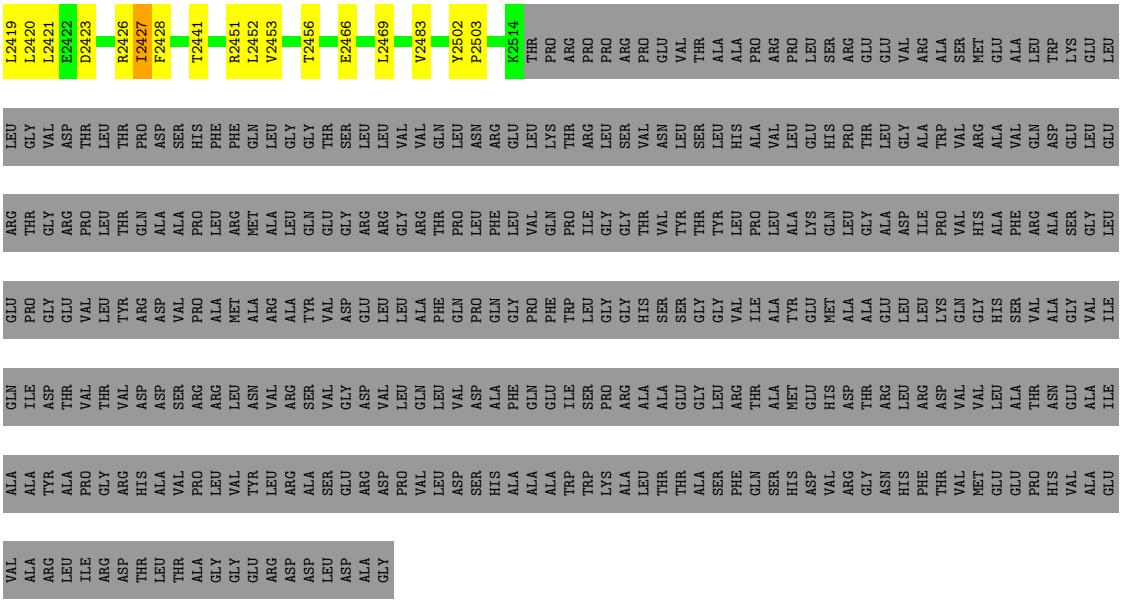
- Molecule 1: Linear gramicidin synthase subunit C

Chain B:





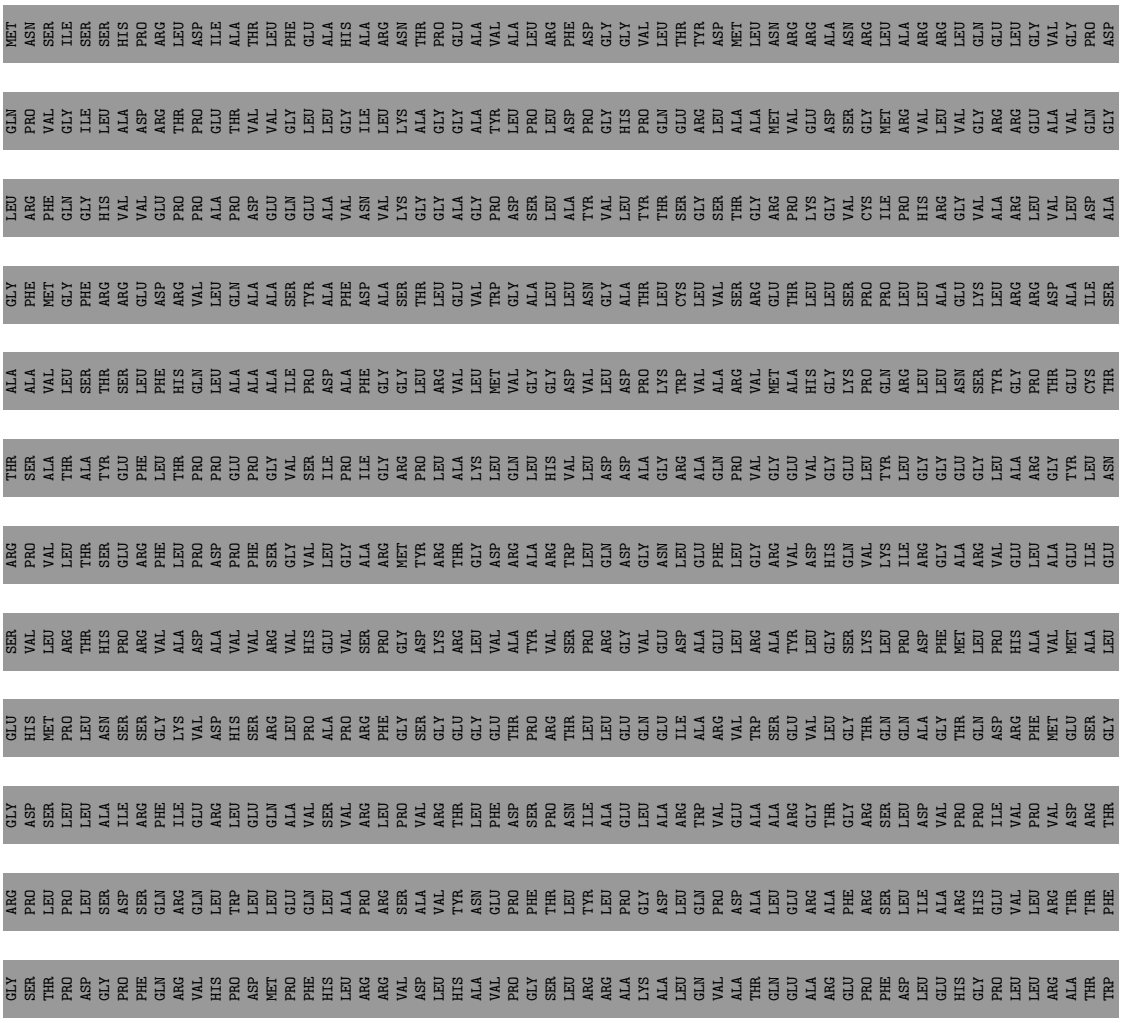

GLY ALA SER LEU PHE MET THR MET LEU SER VAL PHE GLY ALA LEU LEU HIS ARG TYR SER GLY ALA GLU ASP LEU VAL VAL GLY GLY ALA PHE SER GLY LEU PRO LEU ARG LEU ARG PHE SER GLU GLY LEU
THR VAL ARG GLY LEU LEU GLU GLN VAL ARG ARG VAL CYS LEU GLU ALA ALA LEU GLU HIS GLN ASP ALA PRO LEU VAL ARG ILE VAL GLU GLU ALA VAL ASN PRO ALA ARG ILE ALA VAL PRO TRP
ARG VAL GLU PRO HIS ASP VAL ASP THR GLY THR SER LYS LEU ASP LEU SER ILE GLU HIS GLN ALA GLU ASP GLU PRO ASP GLY MET SER VAL ARG TRP GLU TYR ALA LEU ASP VAL PHE GLU PRO TRP MET VAL HIS GLN LEU GLY GLN HIS PHE ASP ALA LEU VAL PRO ASP
PRO GLU GLN LEU LEU SER ALA LEU PRO LEU SER GLU ALA GLN SER GLN VAL LEU ALA TRP ALA HIS GLY PRO ALA ARG GLU VAL ALA HIS CYS LEU HIS HIS PRO PHE GLU ALA GLN VAL GLU ARG THR PRO ALA ARG ILE ALA PRO ALA ALA LEU VAL PHE GLU ALA PRO ARG PRO LEU
SER TYR ARG ALA LEU GLU ALA ASN ARG LEU ALA HIS HIS LEU ILE SER GLN GLY VAL LEU ALA ASP PHE VAL ALA GLN ILE ILE THR LEU LEU LEU ALA LEU LYS ALA GLY ALA PHE SER LEU ASP PRO ALA TYR PRO ARG
ALA ARG LEU GLU PHE MET ALA ARG ASP ALA ALA LEU ALA ALA LEU ARG LEU ILE LEU ALA ALA GLN LEU MET ASP GLY MET GLY VAL PRO VAL VAL GLN LEU GLU GLY VAL ALA GLY GLU ASP ALA PRO ARG ILE HIS VAL THR GLY ASP ALA LEU VAL PHE GLU ALA ARG LEU
THR SER GLY SER THR GLY GLN PRO LYS GLY VAL CYS ILE GLY HIS ARG SER ALA VAL HIS LEU THR GLU THR VAL ALA GLY PHE GLY PHE ALA PRO GLY GLN ARG GLU VAL ALA ALA SER ASP PHE GLY PHE ALA ALA ARG TYR GLY PHE ASP PHE SER VAL ALA ALA GLU ILE PHE PRO THR LEU SER SER GLY ALA
THR LEU TYR LEU MET GLY GLN GLU ASP VAL ALA ALA GLY ALA ALA ASP PHE LEU GLU THR HIS ARG ILE HIS THR ALA ALA MET PHE THR PRO SER ALA LEU GLN ARG LEU ALA SER MET PRO TRP ARG ALA LEU PRO ASP LEU LYS THR LEU LEU ALA ALA ILE GLY GLY GLU GLU LEU PRO ALA LEU ARG LEU
VAL ASP THR TRP ALA PRO GLY ARG PHE ILE GLN VAL TYR GLY PRO THR GLU ALA THR VAL PHE THR THR THR ALA GLU CYS VAL ALA GLY ASP GLY PRO TYR PRO ILE GLY PRO LEU PRO LEU GLY LEU PRO VAL PRO VAL GLY VAL
ARG GLY ALA LEU TYR ILE GLY GLY LYS GLY LEU ALA HIS GLY TYR LEU HIS GLU ARG PRO GLU GLU LEU ASP ALA GLU ARG PHE ILE HIS PRO HIS PRO PHE SER ALA GLU PRO GLY ALA ARG LEU TYR LYS SER GLY ASP ILE ALA SER HIS ARG PRO GLY TYR VAL LEU LEU LEU ASP GLU THR GLY GLY ILE PRO ASP PHE HIS GLY ARG SER
ASP ARG GLN LEU LYS LEU ARG GLY GLU ILE GLU ALA ALA LEU GLU ARG GLN HIS PRO ASP VAL ARG ASP ALA VAL GLU GLU PRO ARG LEU ILE ILE GLU ALA VAL LEU PRO ARG GLU ASP ALA ALA VAL THR PRO ALA PHE LYS GLU SER
LEU GLY LYS THR LEU PRO PRO HIS MET ILE PRO ARG GLU TRP VAL LEU LEU GLU ALA PHE PRO MET GLY PRO THR GLY LYS LEU ASP ARG ASN VAL LEU PRO LEU PRO LEU PRO SER VAL LYS ALA PRO SER PRO ALA ALA PRO GLU SER SER VAL THR GLU ARG GLU LYS ALA LEU GLU ARG ILE TRP
CYS ARG ILE LEU GLY VAL GLU ARG VAL GLY HIS ARG GLN SER ALA LEU ALA SER GLN GLU LEU ASP ILE ARG VAL SER MET ALA THR LEU PHE GLN PHE PRO THR LEU GLU GLU PHE GLN PHE PRO THR LEU LEU ALA ALA LEU ARG HIS ASP ILE ALA
ASP SER THR VAL GLN PRO VAL THR PRO GLU PRO THR ARG SER SER ASP SER I1642 A1643 T1647 P1652 W1661 V1665 R1668 R1673 R1676 L1689 L1701 P1724 M1728 W1734 Y1742 F1771 L1774 Y1781 R1782 S1783 I1784 L1785
L1800 G1801 A1806 T1811 S1814 T1815 S1816 F1843 H1852 I1857 P1860 D1861 D1868 A1869 K1870 G1873 S1878 V1883 K1886 I1898 N1909 D1910 G1911 D1912 F1917 E1923 R1926 T1930 A1940 V1946 H1949 G1950 T1951 A1952 T1953 P1964 L1955 L1964
R1965 R1971 E1975 P1976 K1984 S1985 N1986 V1987 G1988 H1989 S1992 V1996 H2021 P2022 E2023 A2024 R2028 S2029 P2030 F2031 S2035 W2040 R2048 F2055 N2061 L2086 S2095 R2099 R2100 L2101 E2106 R2107 H2108 C2135 A2141 I2142 D2148 A2155 P2159
E2160 Q2171 M2175 W2179 F2197 R2206 L2209 L2210 T2211 D2212 E2213 R2214 E2219 E2220 A2221 L2222 R2223 A2231 S2240 L2243 L2248 T2251 L2254 L2266 S2271 L2272 E2273 Q2274 A2275 V2276 L2281 L2285 S2292 L2295 A2296 V2297 P2298 L2299 S2300 E2301
L2304 A2316 V2317 N2318 Q2322 C2323 V2324 V2325 S2326 F2335 L2339 R2340 V2344 R2345 T2346 K2347 G2354 F2355 L2359 A2363 M2364 A2371 R2372 S2373 M2374 L2383 L2384 W2391 L2392 T2393 A2394 D2395 H2398 D2399 R2400 A2404 R2405 H2406 L2407 R2408 H2409 R2412 F2413 L2417 E2418

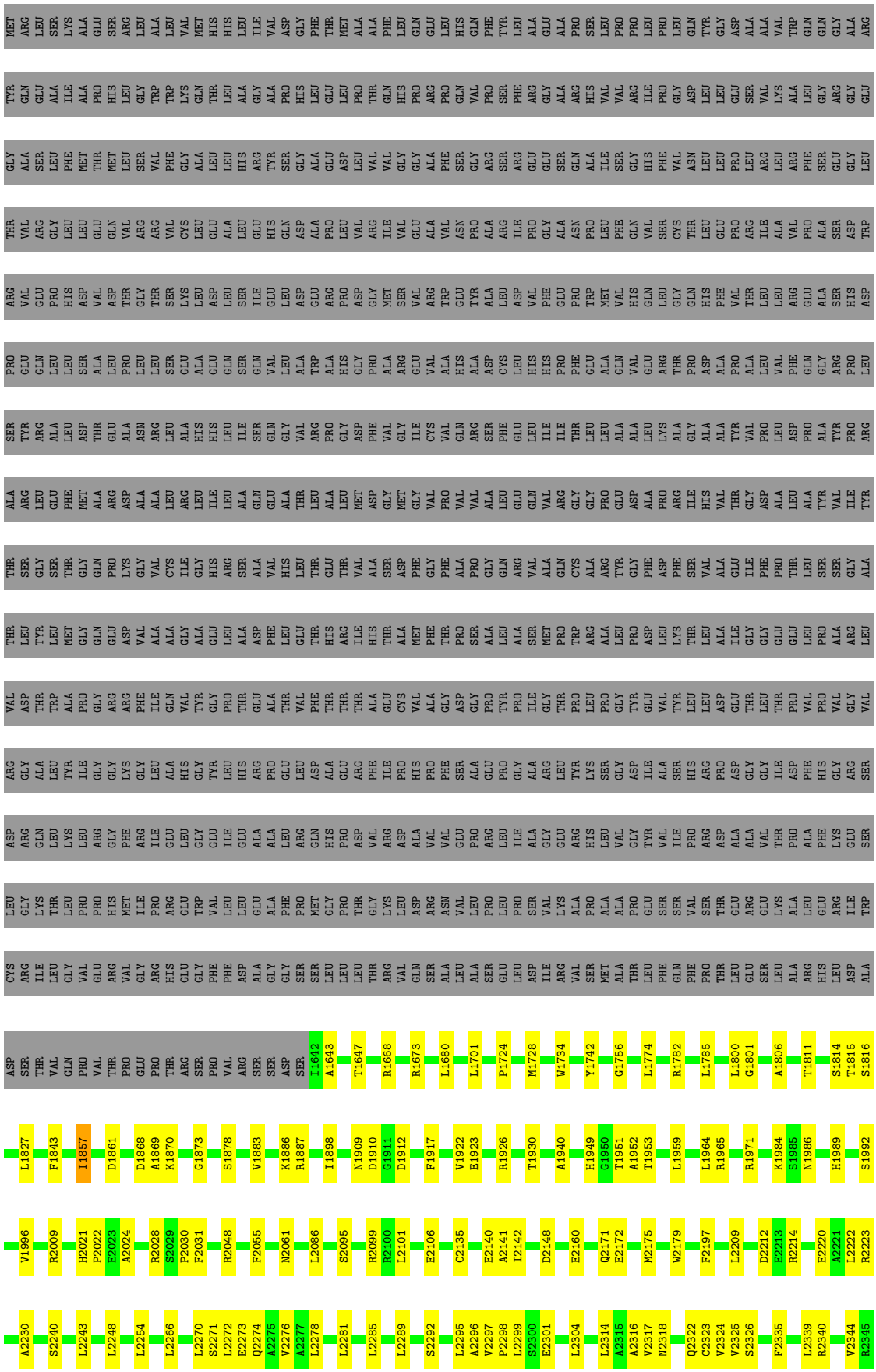


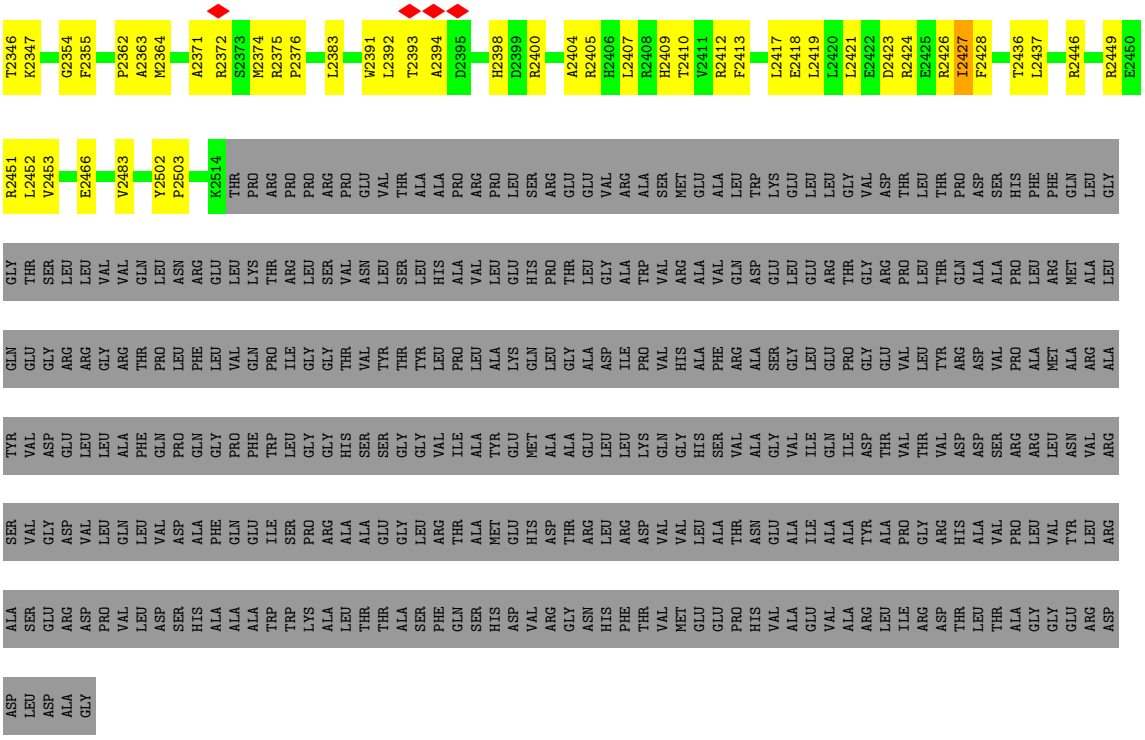
• Molecule 1: Linear gramicidin synthase subunit C

Chain A:






MET ARG LEU SER LYS ALA GLU SER ARG LEU ALA LEU VAL MET HIS HIS LEU ILE VAL ASP GLY PHE THR MET ALA ALA PHE LEU PRO PRO LEU PRO LEU GLN TYR GLY ASP ALA ALA VAL TRP GLN GLN ALA
TYR GLN GLU ALA ILE ALA PRO HIS LEU GLY GLN TRP LYS GLN THR LEU ALA GLY ALA PRO HIS LEU GLU GLU LEU PRO THR GLN LEU GLY GLY TRP PRO ARG PRO GLN VAL PRO SER PHE ARG GLY GLN ILE PRO GLY ASP LEU LEU GLU SER VAL LYS ALA LEU GLY ARG GLU
GLY ALA SER LEU PHE MET THR MET LEU SER VAL PHE GLY ALA LEU LEU HIS ARG TYR SER GLY ALA GLU ASP GLY ALA SER GLN ALA ILE SER GLY HIS PHE VAL ASN LEU LEU LEU PRO LEU ARG ARG LEU ARG PHE SER GLU GLY LEU
THR VAL ARG GLY LEU LEU GLU GLN VAL ARG VAL CYS LEU GLU ALA LEU GLU HIS GLN ASP ALA PRO LEU VAL ARG ILE VAL GLY GLU GLY ALA THR LEU GLU ALA LEU LEU GLU ILE PRO GLY GLY ALA ASN PRO LEU PHE GLN VAL SER CYS THR LEU GLU PRO ARG ILE ALA LEU ASP ASP TRP
ARG VAL GLU PRO HIS ASP VAL ASP THR GLY THR SER LYS LEU ASP LEU SER ILE GLU LEU ASP GLU ARG PRO ASP GLY MET SER VAL ARG TRP ALA LEU ASP VAL LYS LEU ASP PRO TRP PRO MET VAL HIS GLN LEU GLY GLN HIS LEU ASP ALA PHE GLU VAL ASP PRO ARG THR PRO GLU ALA GLN VAL GLU ARG THR PRO ILE ALA ALA ASP ALA ILE HIS GLN VAL ALA ALA LEU LYS ALA GLY ALA ILE HIS VAL ALA THR GLY GLY ASP ALA PRO ARG ILE HIS VAL GLY GLY ALA
PRO GLU GLN LEU LEU SER ALA LEU PRO LEU LEU SER GLN SER ILE GLU VAL LEU LEU ALA HIS GLY PRO ALA GLN GLU VAL ALA HIS HIS PRO PHE GLU ALA GLN VAL GLU ARG THR PRO ALA ASP PRO ALA LEU ALA ALA PHE GLY GLN ALA ALA PRO ALA LEU ALA LEU VAL PHE GLN GLY ALA SER HIS PRO
SER TYR ARG ALA LEU ASP THR GLU ALA GLY ASN GLN ILE LEU ILE SER GLN GLY VAL ALA ILE THR LEU LEU LEU ALA ALA LEU LYS ALA GLY ALA ALA TYR LEU VAL PRO ALA TYR PRO ARG
ALA ARG LEU GLU PHE MET ALA ARG ASP ALA ALA ALA LEU ILE LEU ALA ALA GLN GLU ALA LEU THR ALA LEU ALA LEU MET ASP GLY MET GLY VAL PRO VAL VAL ALA LEU GLU GLY GLN ALA ARG GLY GLY PRO GLU ASP ALA PRO ARG ILE HIS VAL THR ALA GLY ASP ALA LEU LEU ALA ALA TYR VAL ILE TYR
THR SER GLY SER THR GLY GLN PRO LYS GLY VAL CYS ILE GLY HIS ARG SER ALA VAL HIS LEU THR GLU THR VAL ALA SER ASP PHE GLY PHE GLY PHE ALA PRO GLY GLN CYS ALA ARG TYR GLY PHE ASP PHE SER VAL ALA ALA GLU ILE ILE PHE PHE ALA GLN CYS ALA ARG TYR GLY PHE ASP PHE SER VAL ALA ALA GLU ILE ILE PHE PRO THR LEU LEU SER GLY SER GLY ALA
THR LEU TYR LEU MET GLY GLN GLU ASP VAL ALA ALA GLY ALA GLU LEU ASP PHE LEU LEU GLU THR HIS ARG ILE HIS THR ALA MET MET PHE THR PRO SER ALA LEU LEU PRO ASP LEU LYS THR LEU ALA LEU ILE GLY GLY GLY GLU GLU LEU PRO LEU ARG ALA ARG LEU
VAL ASP THR TRP ALA PRO GLY ARG GLY GLY ARG ARG PHE ILE GLN VAL TYR GLY PRO GLY HIS ALA VAL PHE PHE THR THR ALA GLU GLY ASP GLY PRO TYR PRO LEU ILE GLY THR PRO LEU ALA ARG GLY GLY VAL
ARG GLY ALA LEU TYR ILE GLY GLY LYS GLY LEU ALA HIS GLY TYR GLY LEU GLU ALA GLU LEU ASP ALA GLU GLY PRO HIS PRO PHE ILE PRO HIS ALA PRO GLY PHE SER ALA GLU PRO LEU ASP PRO ALA GLY PRO GLY GLY ARG GLY PHE SER GLY TYR ASP ILE ALA SER LEU HIS PRO ARG ARG ASP GLY GLY ARG SER
ASP ARG GLN LEU LYS LEU ARG PHE ILE GLU GLU ALA ALA LEU ARG GLN HIS PRO ASP VAL ARG ASP ALA VAL VAL GLU PRO LEU PRO ARG ASP ALA ALA VAL THR LEU ILE GLU LEU ALA ASP ALA ILE PRO ARG ARG ARG ILE LEU
LEU GLY LYS THR LEU PRO PRO HIS MET ILE PRO ARG GLU TRP VAL LEU GLU GLU ALA PHE PRO MET GLY PRO THR GLY LYS LEU ASP ARG ASP VAL VAL LEU PRO LEU PRO LEU ARG ASN VAL LEU GLU PRO ARG ALA ALA VAL THR PRO LEU ILE ALA PRO ALA ALA PRO GLU SER ILE VAL THR HIS LEU ILE LEU ALA ALA LEU ILE TRP
CYS ARG ILE LEU GLY VAL GLU ARG VAL GLY HIS GLU GLY PHE PHE ASP ALA GLY GLY SER SER SER ASP SER I1642 A1643 T1647 R1668 R1673 L1680 L1701 P1724 M1728 W1734 Y1742 G1756 L1774 R1782 L1785 L1800 G1801 A1806 T1811 S1814 T1815 S1816
L1827 F1843 I1857 D1861 D1868 A1869 K1870 G1873 S1878 V1883 K1886 R1887 I1898 N1909 D1910 G1911 D1912 F1917 V1922 E1923 R1926 T1930 A1940 H1949 G1950 T1951 A1952 T1953 L1959 L1964 R1965 R1971 K1984 S1985 N1986 H1989 S1992
V1996 R2009 H2021 P2022 E2023 A2024 R2028 S2029 P2030 F2031 R2048 F2055 N2061 L2086 S2095 R2099 R2100 L2101 E2106 C2135 E2140 A2141 I2142 D2148 E2160 Q2171 E2172 M2175 W2179 F2197 L2209 D2212 E2213 R2214 E2220 M2221 L2222 R2223
A2230 S2240 L2243 L2248 L2254 L2266 L2270 S2271 L2272 E2273 Q2274 A2275 V2276 A2277 L2278 L2281 L2285 L2289 S2292 L2295 A2296 V2297 P2298 L2299 S2300 E2301 L2304 L2314 A2315 A2316 V2317 N2318 Q2322 C2323 V2324 V2325 S2326 F2335 L2339 R2340 V2344 R2345


T2346 K2347 G2354 F2355 P2362 A2363 M2364 A2371 R2372 S2373 M2374 R2375 P2376 L2383 W2391 L2392 T2393 A2394 D2395 H2398 D2399 R2400 A2404 R2405 H2406 L2407 R2408 H2409 T2410 V2411 R2412 F2413 L2417 E2418 L2419 L2420 L2421 E2422 D2423 R2424 E2425 R2426 I2427 F2428 T2436 L2437 R2446 R2449 E2450
R2451 L2452 V2453 E2466 V2483 Y2502 P2503 K2514 THR PRO ARG PRO PRO ARG PRO GLU VAL THR ALA ALA PRO ARG PRO LEU SER ARG GLU GLU VAL ARG ALA SER MET GLU ALA LEU TRP LYS GLU LEU LEU GLY VAL ASP THR LEU THR PRO ASP SER HIS PHE PHE GLN LEU GLY
GLY THR SER LEU LEU VAL VAL GLN LEU ASN ARG GLU LEU LYS THR ARG LEU SER VAL ASN LEU SER LEU HIS ALA ALA PRO VAL LEU GLU HIS PRO THR LEU GLY ALA ALA TRP VAL ARG ALA VAL GLN ASP GLU LEU GLU LEU ARG THR GLY VAL ARG PRO LEU THR GLN ALA ALA PRO LEU ARG MET ALA LEU
GLN GLU GLY ARG ARG GLY ARG THR PRO LEU PHE LEU VAL GLN PRO ILE GLY GLY THR VAL TYR THR TYR LEU PRO LEU ALA LYS GLN LEU GLY ALA ASP ILE PRO VAL HIS ALA PHE ARG ALA SER GLY LEU GLU PRO GLY GLU VAL LEU TYR ARG ASP VAL PRO ALA MET ALA ARG ALA
TYR VAL ASP GLU LEU LEU ALA PHE GLN PRO GLN GLY PRO PHE TRP LEU GLY GLY HIS SER SER GLY GLY VAL ILE ALA TYR GLU MET ALA ALA GLU LEU LEU LYS GLN GLY HIS SER VAL ALA GLY VAL ILE GLN ILE ASP THR VAL THR VAL ASP SER ARG ARG LEU ASN VAL ARG
SER VAL GLY ASP VAL LEU GLN LEU VAL ASP ALA PHE GLN GLU ILE SER PRO ARG ALA ALA GLU GLY LEU ARG THR ALA MET GLU HIS ASP THR ARG LEU ARG ASP VAL VAL LEU ALA THR ASN GLU ALA ILE ALA ALA TYR ALA PRO GLY ARG HIS ALA VAL PRO LEU VAL TYR LEU ARG
ALA SER GLU ARG ASP PRO VAL LEU ASP SER HIS ALA ALA ALA TRP TRP LYS ALA LEU THR THR ALA SER PHE GLN SER HIS ASP VAL ARG GLY ASN HIS PHE THR VAL MET GLU GLU PRO HIS VAL ALA GLU VAL ALA ARG LEU ILE ARG ASP THR LEU THR ALA GLY GLY GLU ARG ASP
ASP LEU ASP ALA GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.496	Depositor
Minimum map value	-0.806	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	284.8, 284.8, 284.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	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	0.21	0/6690	0.36	1/9109 (0.0%)
1	B	0.22	0/6690	0.37	1/9109 (0.0%)
All	All	0.21	0/13380	0.37	2/18218 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1782	ARG	N-CA-C	-5.22	107.57	114.31
1	A	1782	ARG	N-CA-C	-5.03	107.83	114.31

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	A	6541	0	6494	112	0
1	B	6541	0	6494	127	0
All	All	13082	0	12988	230	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.

All (230) 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:2219:GLU:HG3	1:B:2223:ARG:HH12	1.29	0.95
1:A:2405:ARG:HB3	1:A:2409:HIS:HE1	1.43	0.81
1:B:1965:ARG:HH12	1:B:2028:ARG:HG3	1.47	0.79
1:B:2171:GLN:HG3	1:B:2222:LEU:HD12	1.63	0.79
1:A:2171:GLN:HG3	1:A:2222:LEU:HD12	1.64	0.78
1:B:1964:LEU:HD22	1:B:2031:PHE:HZ	1.50	0.75
1:B:2398:HIS:O	1:B:2400:ARG:NH1	2.19	0.75
1:A:2220:GLU:HA	1:A:2223:ARG:HG3	1.67	0.75
1:A:2248:LEU:HD21	1:A:2483:VAL:HG22	1.69	0.74
1:A:1965:ARG:HH12	1:A:2028:ARG:HG3	1.51	0.74
1:A:2398:HIS:O	1:A:2400:ARG:NH1	2.21	0.73
1:B:2248:LEU:HD21	1:B:2483:VAL:HG22	1.71	0.71
1:A:2428:PHE:HB2	1:A:2453:VAL:HG13	1.74	0.69
1:B:2384:LEU:HD21	1:B:2419:LEU:HD22	1.73	0.69
1:A:1643:ALA:HB1	1:A:1898:ILE:HG23	1.75	0.69
1:B:1964:LEU:HD22	1:B:2031:PHE:CZ	2.29	0.68
1:B:1643:ALA:HB1	1:B:1898:ILE:HG23	1.75	0.67
1:B:2175:MET:HG2	1:B:2209:LEU:HD22	1.76	0.66
1:B:1909:ASN:HD22	1:A:1806:ALA:HB3	1.62	0.65
1:A:2297:VAL:HG12	1:A:2299:LEU:H	1.62	0.65
1:A:2160:GLU:OE2	1:A:2426:ARG:NH2	2.31	0.64
1:B:2423:ASP:O	1:B:2451:ARG:NH2	2.30	0.64
1:B:2219:GLU:HG3	1:B:2223:ARG:NH1	2.09	0.63
1:B:2297:VAL:HG12	1:B:2299:LEU:H	1.62	0.63
1:A:2175:MET:HG2	1:A:2209:LEU:HD22	1.78	0.63
1:A:2423:ASP:O	1:A:2451:ARG:NH2	2.31	0.63
1:B:2316:ALA:HB3	1:B:2324:VAL:HB	1.81	0.62
1:A:1742:TYR:OH	1:A:1886:LYS:NZ	2.32	0.62
1:A:2383:LEU:HD11	1:A:2392:LEU:HD23	1.82	0.62
1:B:1742:TYR:OH	1:B:1886:LYS:NZ	2.32	0.61
1:A:1964:LEU:HD22	1:A:2031:PHE:CZ	2.35	0.61
1:A:2417:LEU:O	1:A:2421:LEU:HD12	1.99	0.61
1:B:2417:LEU:O	1:B:2421:LEU:HD12	2.00	0.61
1:B:2428:PHE:HB2	1:B:2453:VAL:HG13	1.82	0.61
1:A:2095:SER:OG	1:A:2148:ASP:OD2	2.17	0.60
1:A:1843:PHE:H	1:A:1878:SER:HB3	1.67	0.60
1:B:1843:PHE:H	1:B:1878:SER:HB3	1.67	0.60
1:B:2405:ARG:HB3	1:B:2409:HIS:HE1	1.65	0.60
1:A:2271:SER:N	1:A:2274:GLN:OE1	2.33	0.60
1:A:2427:ILE:HG22	1:A:2452:LEU:HB3	1.83	0.60
1:B:1676:ARG:HG3	1:B:1689:LEU:HD23	1.84	0.60
1:B:2271:SER:N	1:B:2274:GLN:OE1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2405:ARG:HB3	1:B:2409:HIS:CE1	2.37	0.60
1:A:2316:ALA:HB3	1:A:2324:VAL:HB	1.83	0.60
1:A:2317:VAL:HB	1:A:2412:ARG:HG2	1.85	0.59
1:B:2281:LEU:O	1:B:2285:LEU:HG	2.03	0.58
1:B:2383:LEU:HD11	1:B:2392:LEU:HD23	1.85	0.58
1:B:2426:ARG:HD3	1:B:2428:PHE:HE2	1.67	0.58
1:B:1806:ALA:HB3	1:A:1909:ASN:HD22	1.67	0.58
1:A:2394:ALA:O	1:A:2398:HIS:NE2	2.36	0.58
1:A:1673:ARG:NH2	1:A:1861:ASP:O	2.37	0.57
1:B:2160:GLU:OE1	1:B:2426:ARG:NH2	2.37	0.57
1:A:2326:SER:OG	1:A:2355:PHE:O	2.23	0.57
1:A:1964:LEU:HD22	1:A:2031:PHE:HZ	1.68	0.56
1:A:2418:GLU:HB2	1:A:2446:ARG:NH1	2.20	0.56
1:A:2426:ARG:HD3	1:A:2428:PHE:HE1	1.70	0.56
1:A:1873:GLY:N	1:A:1952:ALA:O	2.38	0.56
1:A:2021:HIS:HB3	1:A:2024:ALA:HB2	1.88	0.56
1:B:1673:ARG:NH2	1:B:1861:ASP:O	2.39	0.56
1:A:2372:ARG:HD3	1:A:2400:ARG:HH21	1.71	0.56
1:B:2055:PHE:HD1	1:B:2061:ASN:HB3	1.71	0.56
1:A:2298:PRO:HD2	1:A:2344:VAL:HG13	1.88	0.56
1:B:2326:SER:OG	1:B:2355:PHE:O	2.24	0.55
1:B:1873:GLY:N	1:B:1952:ALA:O	2.39	0.55
1:B:2243:LEU:HD22	1:B:2248:LEU:HD12	1.88	0.55
1:B:2271:SER:O	1:B:2273:GLU:N	2.39	0.55
1:B:2394:ALA:O	1:B:2398:HIS:NE2	2.39	0.55
1:A:2243:LEU:HD22	1:A:2248:LEU:HD12	1.88	0.55
1:A:2340:ARG:O	1:A:2340:ARG:NH1	2.36	0.55
1:A:2271:SER:O	1:A:2273:GLU:N	2.39	0.55
1:B:2021:HIS:HB3	1:B:2024:ALA:HB2	1.88	0.55
1:B:2355:PHE:HE2	1:B:2407:LEU:HD12	1.72	0.54
1:A:1816:SER:OG	1:A:1992:SER:O	2.25	0.54
1:B:2340:ARG:O	1:B:2340:ARG:NH1	2.36	0.54
1:A:2197:PHE:CE1	1:A:2276:VAL:HG13	2.42	0.54
1:B:2371:ALA:HB1	1:B:2400:ARG:HG3	1.90	0.54
1:A:2055:PHE:HD1	1:A:2061:ASN:HB3	1.71	0.54
1:B:2372:ARG:HD3	1:B:2400:ARG:HH21	1.73	0.54
1:A:2295:LEU:HD22	1:A:2325:VAL:HB	1.90	0.54
1:B:1811:THR:O	1:B:1811:THR:OG1	2.24	0.54
1:B:2298:PRO:HD2	1:B:2344:VAL:HG13	1.89	0.54
1:B:2099:ARG:HH21	1:B:2148:ASP:HB2	1.73	0.53
1:B:2212:ASP:O	1:B:2214:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2299:LEU:HD13	1:A:2304:LEU:HD13	1.90	0.53
1:B:1668:ARG:O	1:B:1986:ASN:ND2	2.42	0.53
1:B:2427:ILE:HG22	1:B:2452:LEU:HB3	1.91	0.53
1:A:2436:THR:HG22	1:A:2437:LEU:HD23	1.91	0.53
1:B:1816:SER:OG	1:B:1992:SER:O	2.25	0.52
1:A:2212:ASP:O	1:A:2214:ARG:NH1	2.42	0.52
1:A:2254:LEU:HG	1:A:2413:PHE:HE1	1.74	0.52
1:B:2317:VAL:HB	1:B:2412:ARG:HG2	1.91	0.52
1:B:2285:LEU:HD13	1:B:2363:ALA:HB1	1.92	0.52
1:B:2240:SER:HB3	1:B:2266:LEU:HD21	1.91	0.52
1:A:1668:ARG:O	1:A:1986:ASN:ND2	2.43	0.52
1:B:1984:LYS:HE3	1:B:1989:HIS:ND1	2.25	0.52
1:A:2240:SER:HB3	1:A:2266:LEU:HD21	1.91	0.51
1:A:2281:LEU:O	1:A:2285:LEU:HD13	2.09	0.51
1:B:1814:SER:O	1:B:1814:SER:OG	2.28	0.51
1:B:2095:SER:OG	1:B:2148:ASP:OD2	2.19	0.51
1:B:2295:LEU:HD22	1:B:2325:VAL:HB	1.93	0.51
1:B:2206:ARG:HG3	1:B:2210:LEU:HD22	1.93	0.51
1:A:2099:ARG:HH21	1:A:2148:ASP:HB2	1.76	0.51
1:B:1971:ARG:HG3	1:B:2030:PRO:HG3	1.92	0.50
1:A:2179:TRP:CZ2	1:A:2466:GLU:HA	2.47	0.50
1:B:1946:VAL:HG11	1:B:1964:LEU:HD11	1.92	0.50
1:B:2135:CYS:SG	1:B:2141:ALA:HB2	2.52	0.50
1:A:2295:LEU:N	1:A:2325:VAL:O	2.45	0.50
1:A:2391:TRP:NE1	1:A:2419:LEU:HD21	2.27	0.50
1:B:2220:GLU:OE1	1:B:2223:ARG:NH2	2.36	0.50
1:B:2197:PHE:HE1	1:B:2276:VAL:HG22	1.77	0.49
1:B:2299:LEU:HD13	1:B:2304:LEU:HD13	1.92	0.49
1:A:2106:GLU:HG3	1:A:2142:ILE:HD13	1.93	0.49
1:B:1781:TYR:HE2	1:A:1857:ILE:HD11	1.77	0.49
1:B:2295:LEU:N	1:B:2325:VAL:O	2.46	0.49
1:B:2155:ALA:HB3	1:B:2159:PRO:HD3	1.94	0.49
1:B:1926:ARG:O	1:B:1930:THR:HG23	2.13	0.49
1:B:1940:ALA:O	1:B:1971:ARG:NH2	2.42	0.49
1:A:2355:PHE:HE2	1:A:2407:LEU:HD12	1.77	0.49
1:A:1926:ARG:O	1:A:1930:THR:HG23	2.13	0.48
1:B:2179:TRP:CZ2	1:B:2466:GLU:HA	2.48	0.48
1:B:2292:SER:HB2	1:B:2354:GLY:HA3	1.95	0.48
1:A:2371:ALA:HB1	1:A:2400:ARG:HG3	1.95	0.48
1:B:1975:GLU:HG3	1:B:1976:PRO:HD2	1.96	0.48
1:B:2254:LEU:HG	1:B:2413:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2135:CYS:SG	1:A:2141:ALA:HB2	2.53	0.48
1:A:2289:LEU:HD11	1:A:2362:PRO:HG2	1.95	0.48
1:B:1647:THR:HG22	1:B:1883:VAL:HG12	1.96	0.48
1:A:2372:ARG:HH12	1:A:2375:ARG:HD3	1.78	0.48
1:A:1909:ASN:OD1	1:A:1910:ASP:N	2.47	0.48
1:A:1984:LYS:HE3	1:A:1989:HIS:ND1	2.29	0.47
1:A:1965:ARG:NH1	1:A:2028:ARG:HG3	2.25	0.47
1:A:2335:PHE:CD2	1:A:2339:LEU:HD13	2.49	0.47
1:B:2335:PHE:CD2	1:B:2339:LEU:HD13	2.49	0.47
1:A:1647:THR:HG22	1:A:1883:VAL:HG12	1.95	0.47
1:B:2223:ARG:NH1	1:B:2223:ARG:HG3	2.30	0.47
1:A:2285:LEU:HD23	1:A:2363:ALA:HB1	1.96	0.47
1:A:1868:ASP:OD1	1:A:1869:ALA:N	2.47	0.47
1:A:2172:GLU:H	1:A:2175:MET:HE2	1.80	0.47
1:A:2364:MET:HG2	1:A:2404:ALA:HB1	1.96	0.47
1:B:1912:ASP:HB3	1:A:1801:GLY:HA2	1.96	0.47
1:B:2346:THR:OG1	1:B:2347:LYS:N	2.48	0.47
1:B:2391:TRP:NE1	1:B:2419:LEU:HD21	2.30	0.47
1:A:1949:HIS:O	1:A:1984:LYS:HD2	2.14	0.47
1:A:1811:THR:O	1:A:1811:THR:OG1	2.24	0.46
1:B:2502:TYR:CD2	1:B:2503:PRO:HD2	2.51	0.46
1:B:2274:GLN:HG2	1:B:2374:MET:HE2	1.97	0.46
1:B:1949:HIS:O	1:B:1984:LYS:HD2	2.16	0.46
1:B:2107:ARG:NH1	1:B:2108:HIS:HE1	2.13	0.46
1:A:2314:LEU:O	1:A:2410:THR:OG1	2.32	0.46
1:B:1801:GLY:HA2	1:A:1912:ASP:HB3	1.97	0.46
1:A:2292:SER:HB2	1:A:2354:GLY:HA3	1.96	0.46
1:B:1661:TRP:O	1:B:1665:VAL:HG12	2.15	0.45
1:B:1724:PRO:O	1:B:1728:MET:HG3	2.17	0.45
1:B:2160:GLU:HB2	1:B:2251:THR:OG1	2.16	0.45
1:B:2223:ARG:HG3	1:B:2223:ARG:HH11	1.82	0.45
1:B:2456:THR:O	1:B:2456:THR:OG1	2.31	0.45
1:B:2209:LEU:HD11	1:B:2231:ALA:HB1	1.98	0.45
1:B:2106:GLU:HG3	1:B:2142:ILE:HD13	1.97	0.45
1:B:2212:ASP:OD1	1:B:2212:ASP:N	2.34	0.45
1:B:2301:GLU:HB2	1:B:2323:CYS:SG	2.57	0.45
1:B:1868:ASP:OD1	1:B:1870:LYS:HG3	2.17	0.44
1:A:1724:PRO:O	1:A:1728:MET:HG3	2.17	0.44
1:A:2346:THR:OG1	1:A:2347:LYS:N	2.50	0.44
1:B:1868:ASP:OD1	1:B:1869:ALA:N	2.50	0.44
1:B:2400:ARG:N	1:B:2400:ARG:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2301:GLU:HB2	1:A:2323:CYS:SG	2.58	0.44
1:B:1852:HIS:CE1	1:B:1860:PRO:HG3	2.53	0.44
1:B:1734:TRP:HE3	1:B:1800:LEU:HD22	1.83	0.44
1:B:1816:SER:HB3	1:B:1996:VAL:HB	1.99	0.44
1:A:2424:ARG:HA	1:A:2451:ARG:HH22	1.83	0.44
1:B:2372:ARG:HD2	1:B:2372:ARG:HA	1.81	0.44
1:A:2400:ARG:HD2	1:A:2400:ARG:N	2.33	0.44
1:B:2318:ASN:HB2	1:B:2322:GLN:HG2	2.00	0.43
1:A:1816:SER:HB3	1:A:1996:VAL:HB	1.99	0.43
1:A:1868:ASP:OD1	1:A:1870:LYS:HG3	2.18	0.43
1:B:1909:ASN:OD1	1:B:1910:ASP:N	2.51	0.43
1:B:1965:ARG:NH1	1:B:2028:ARG:HG3	2.25	0.43
1:A:1734:TRP:HE3	1:A:1800:LEU:HD22	1.83	0.43
1:A:2296:ALA:HB3	1:A:2347:LYS:H	1.82	0.43
1:A:2295:LEU:HB2	1:A:2325:VAL:H	1.84	0.43
1:B:1898:ILE:H	1:B:1898:ILE:HG13	1.51	0.43
1:A:1922:VAL:HG22	1:A:1959:LEU:HG	2.00	0.43
1:A:2095:SER:O	1:A:2099:ARG:HG2	2.19	0.43
1:A:2140:GLU:H	1:A:2140:GLU:HG2	1.66	0.43
1:B:2021:HIS:ND1	1:B:2022:PRO:HD2	2.34	0.43
1:A:1971:ARG:HG3	1:A:2030:PRO:HG3	2.00	0.43
1:B:1785:LEU:HD22	1:A:1917:PHE:HE2	1.84	0.42
1:A:2197:PHE:HE2	1:A:2230:ALA:HA	1.85	0.42
1:A:2355:PHE:CE2	1:A:2407:LEU:HD12	2.53	0.42
1:B:2428:PHE:CD1	1:B:2441:THR:HG21	2.54	0.42
1:A:2421:LEU:HG	1:A:2428:PHE:CZ	2.55	0.42
1:B:1806:ALA:CB	1:A:1909:ASN:HD22	2.31	0.42
1:B:1857:ILE:HD12	1:B:1857:ILE:H	1.84	0.42
1:B:2095:SER:O	1:B:2099:ARG:HG2	2.18	0.42
1:A:2449:ARG:HD2	1:A:2449:ARG:HA	1.84	0.42
1:B:1701:LEU:HD13	1:B:1728:MET:HE1	2.02	0.42
1:A:2021:HIS:ND1	1:A:2022:PRO:HD2	2.34	0.42
1:A:1923:GLU:OE1	1:A:1926:ARG:NH2	2.48	0.42
1:A:2318:ASN:HB2	1:A:2322:GLN:HG2	2.01	0.42
1:B:1917:PHE:HE2	1:A:1785:LEU:HD22	1.84	0.42
1:A:1951:THR:O	1:A:1953:THR:N	2.48	0.41
1:A:1827:LEU:O	1:A:1887:ARG:NH1	2.43	0.41
1:A:1940:ALA:O	1:A:1971:ARG:NH2	2.46	0.41
1:B:2086:LEU:HD11	1:B:2101:LEU:HD23	2.02	0.41
1:A:1680:LEU:HD23	1:A:1680:LEU:HA	1.94	0.41
1:A:1701:LEU:HD13	1:A:1728:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2270:LEU:HD21	1:A:2278:LEU:HD12	2.01	0.41
1:A:2502:TYR:CD1	1:A:2503:PRO:HD2	2.55	0.41
1:B:2428:PHE:HD1	1:B:2441:THR:HG21	1.86	0.41
1:B:2035:SER:O	1:B:2035:SER:OG	2.35	0.41
1:B:2426:ARG:HD3	1:B:2428:PHE:CE2	2.52	0.41
1:B:1652:PRO:HD2	1:B:1987:VAL:HB	2.03	0.41
1:B:1955:LEU:HD12	1:B:1955:LEU:HA	1.93	0.41
1:B:1781:TYR:CE2	1:A:1857:ILE:HD11	2.55	0.41
1:B:2040:TRP:O	1:B:2048:ARG:NH2	2.54	0.41
1:B:2243:LEU:HD23	1:B:2243:LEU:HA	1.89	0.41
1:A:1756:GLY:HA3	1:A:1815:THR:HG21	2.03	0.41
1:A:1814:SER:O	1:A:1814:SER:OG	2.29	0.41
1:A:2086:LEU:HD11	1:A:2101:LEU:HD23	2.02	0.41
1:B:1701:LEU:HD23	1:B:1701:LEU:HA	1.90	0.40
1:B:2364:MET:HG2	1:B:2404:ALA:HB1	2.03	0.40
1:A:2009:ARG:HD3	1:A:2048:ARG:NH2	2.36	0.40
1:A:2374:MET:O	1:A:2376:PRO:HD3	2.21	0.40
1:B:1923:GLU:OE1	1:B:1926:ARG:NH2	2.54	0.40
1:B:1951:THR:O	1:B:1953:THR:N	2.49	0.40
1:B:1771:PHE:HD1	1:B:1783:SER:HB3	1.86	0.40
1:B:2420:LEU:HD23	1:B:2420:LEU:HA	1.80	0.40
1:B:2451:ARG:HD3	1:B:2451:ARG:HA	1.86	0.40
1:B:2179:TRP:CZ2	1:B:2469:LEU:HD23	2.56	0.40
1:B:2322:GLN:OE1	1:B:2322:GLN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	871/2867 (30%)	813 (93%)	56 (6%)	2 (0%)	43 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	871/2867 (30%)	815 (94%)	54 (6%)	2 (0%)	43 73
All	All	1742/5734 (30%)	1628 (94%)	110 (6%)	4 (0%)	44 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2272	LEU
1	A	2272	LEU
1	B	1774	LEU
1	A	1774	LEU

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	664/2276 (29%)	661 (100%)	3 (0%)	81 85
1	B	664/2276 (29%)	662 (100%)	2 (0%)	86 87
All	All	1328/4552 (29%)	1323 (100%)	5 (0%)	81 86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2359	LEU
1	B	2427	ILE
1	A	1857	ILE
1	A	2393	THR
1	A	2427	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1799	GLN
1	B	1863	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1908	ASN
1	B	2108	HIS
1	B	2406	HIS
1	A	1799	GLN
1	A	1908	ASN
1	A	1986	ASN
1	A	2386	ASN
1	A	2475	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 oligosaccharides 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.

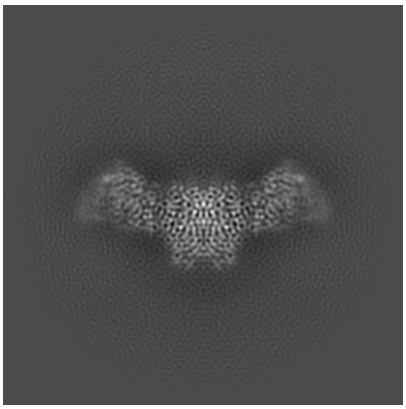
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-81083. These allow visual inspection of the internal detail of the map and identification of artifacts.

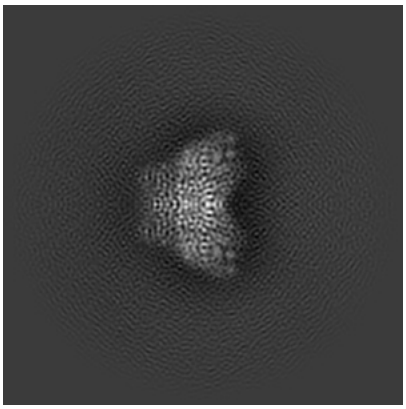
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

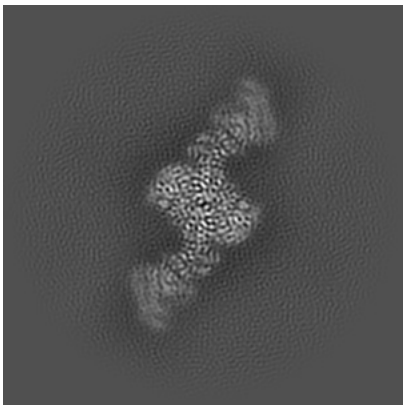
6.1.1 Primary map



X

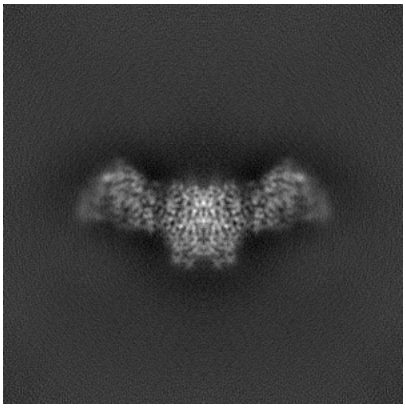


Y

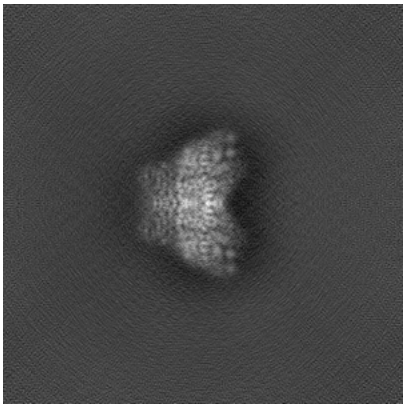


Z

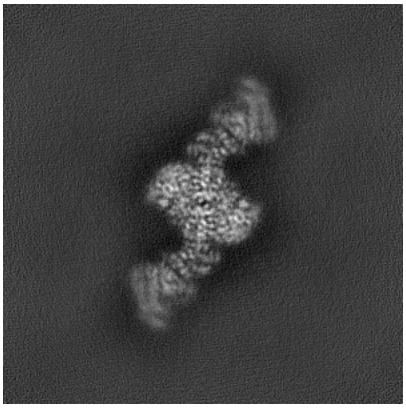
6.1.2 Raw map



X



Y

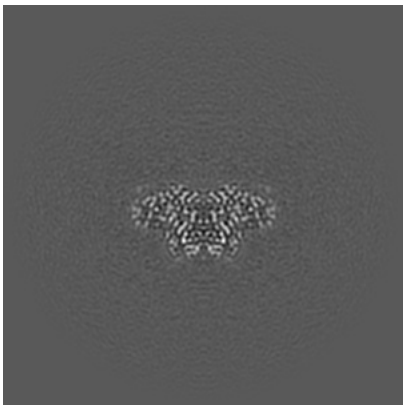


Z

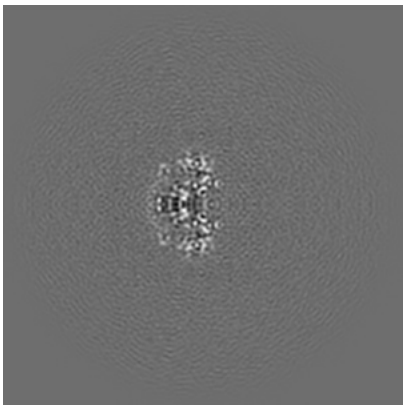
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

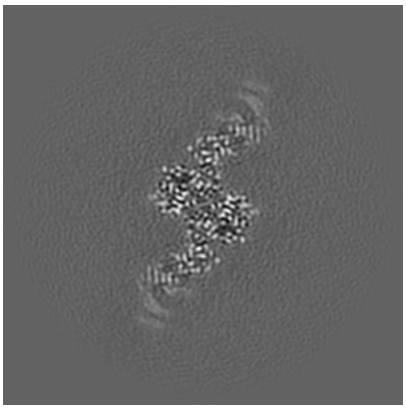
6.2.1 Primary map



X Index: 160

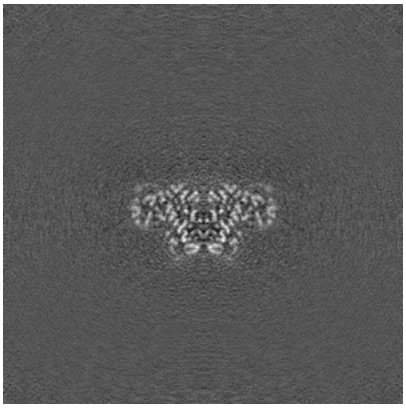


Y Index: 160

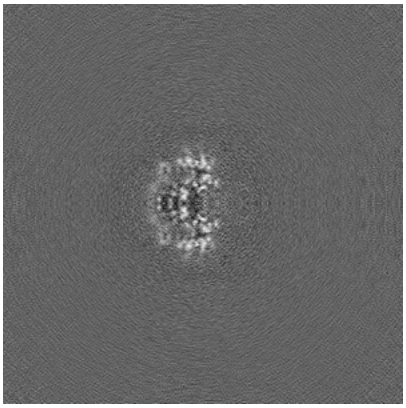


Z Index: 160

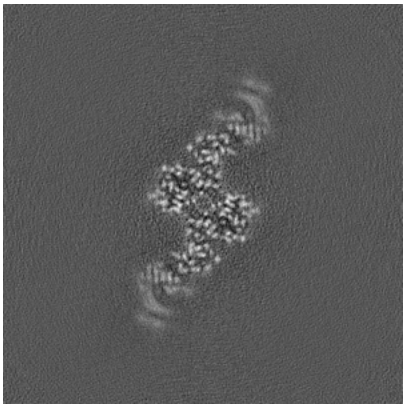
6.2.2 Raw map



X Index: 160



Y Index: 160

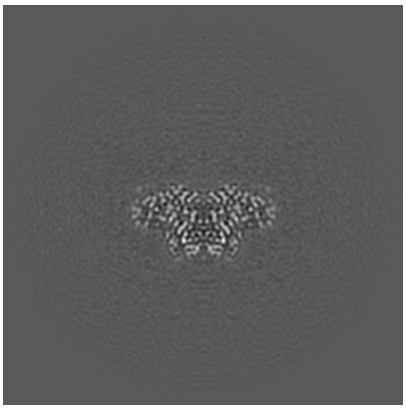


Z Index: 160

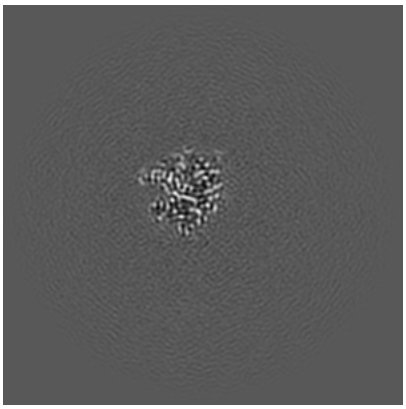
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

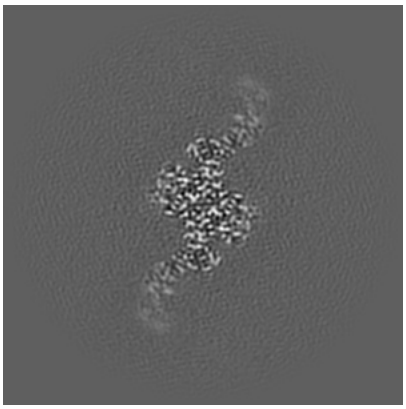
6.3.1 Primary map



X Index: 160

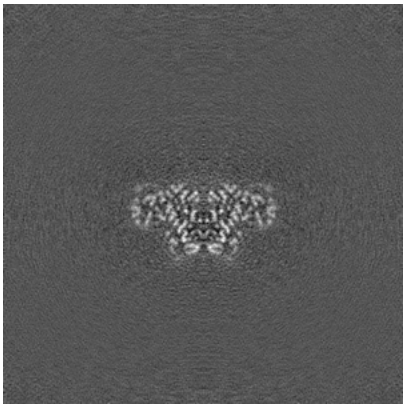


Y Index: 148

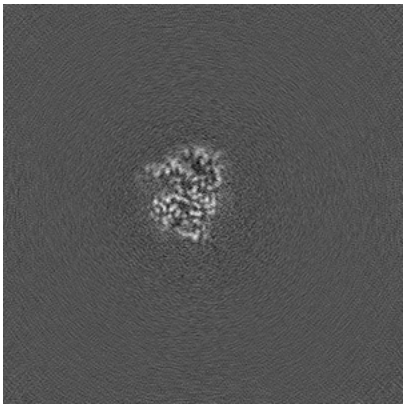


Z Index: 153

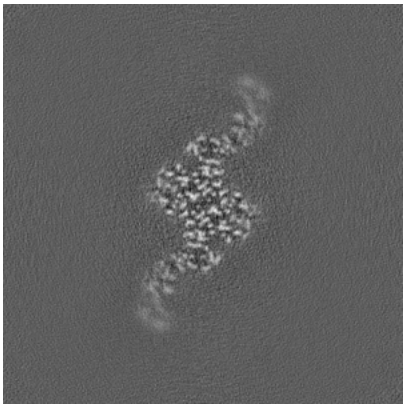
6.3.2 Raw map



X Index: 160



Y Index: 153

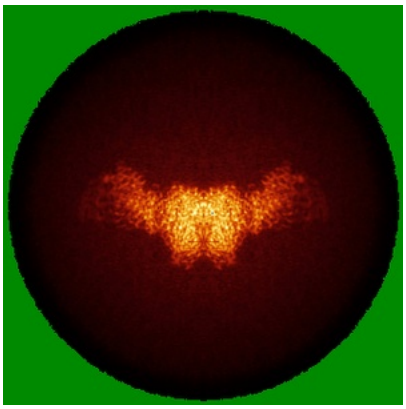


Z Index: 153

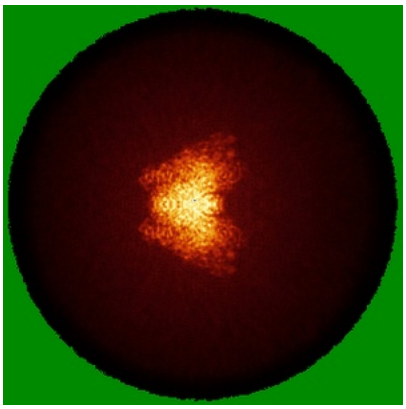
The images above show the largest variance slices of the map in three orthogonal directions.

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

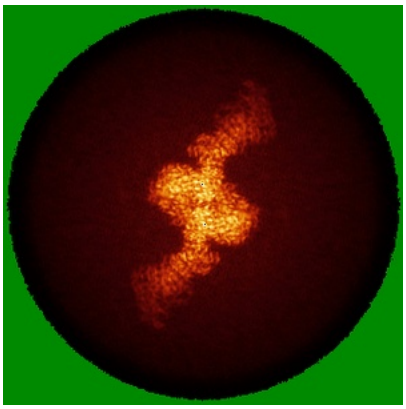
6.4.1 Primary map



X

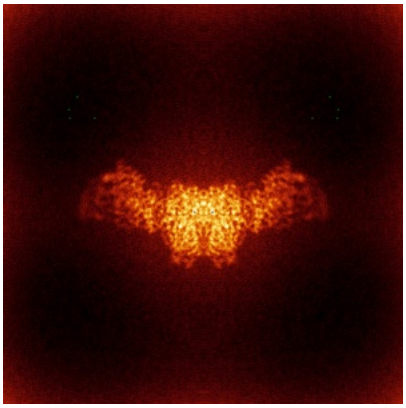


Y

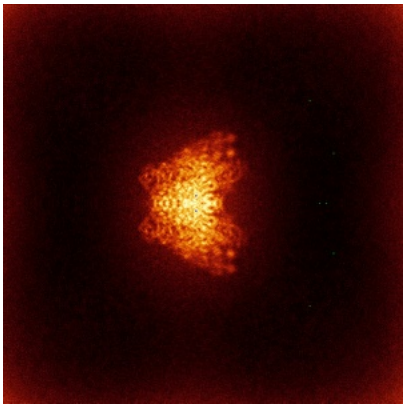


Z

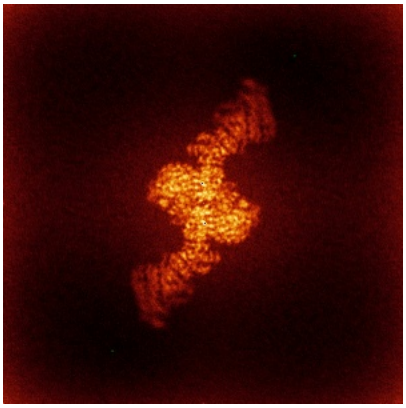
6.4.2 Raw map



X



Y

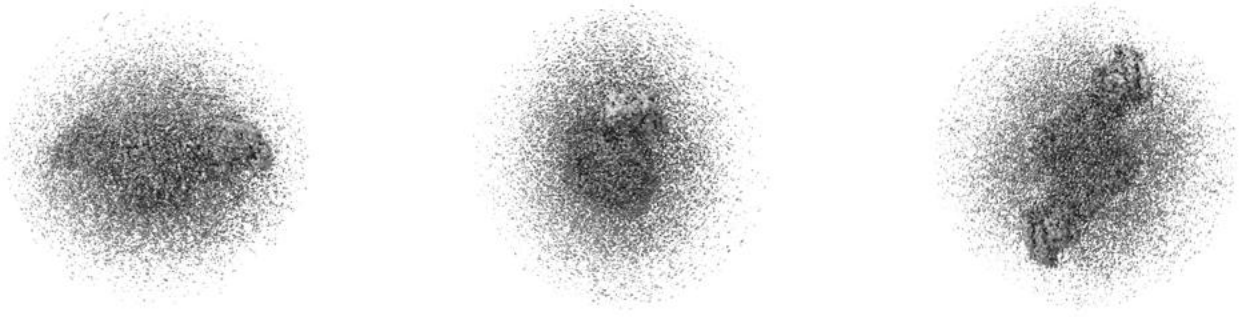


Z

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)

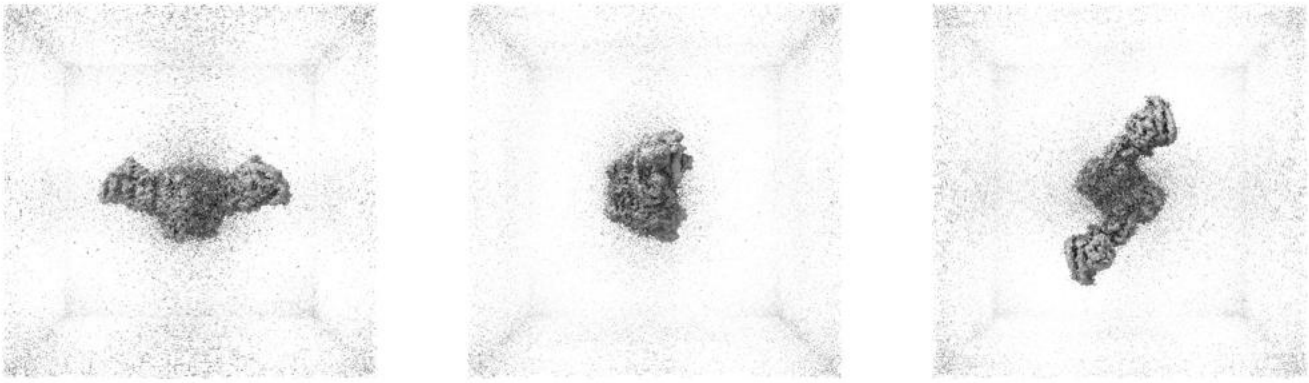
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

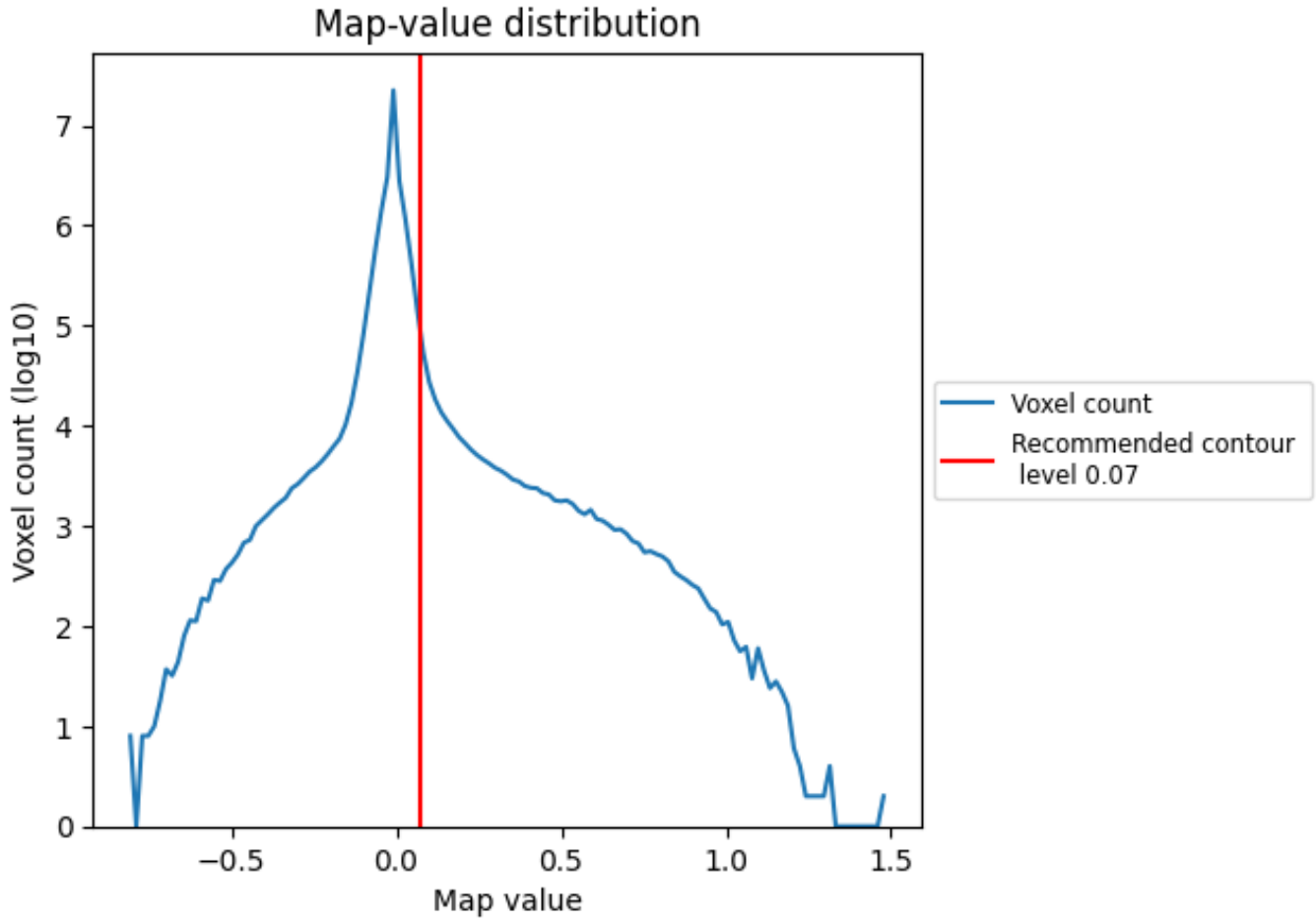
6.6 Mask visualisation (i)

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

7 Map analysis

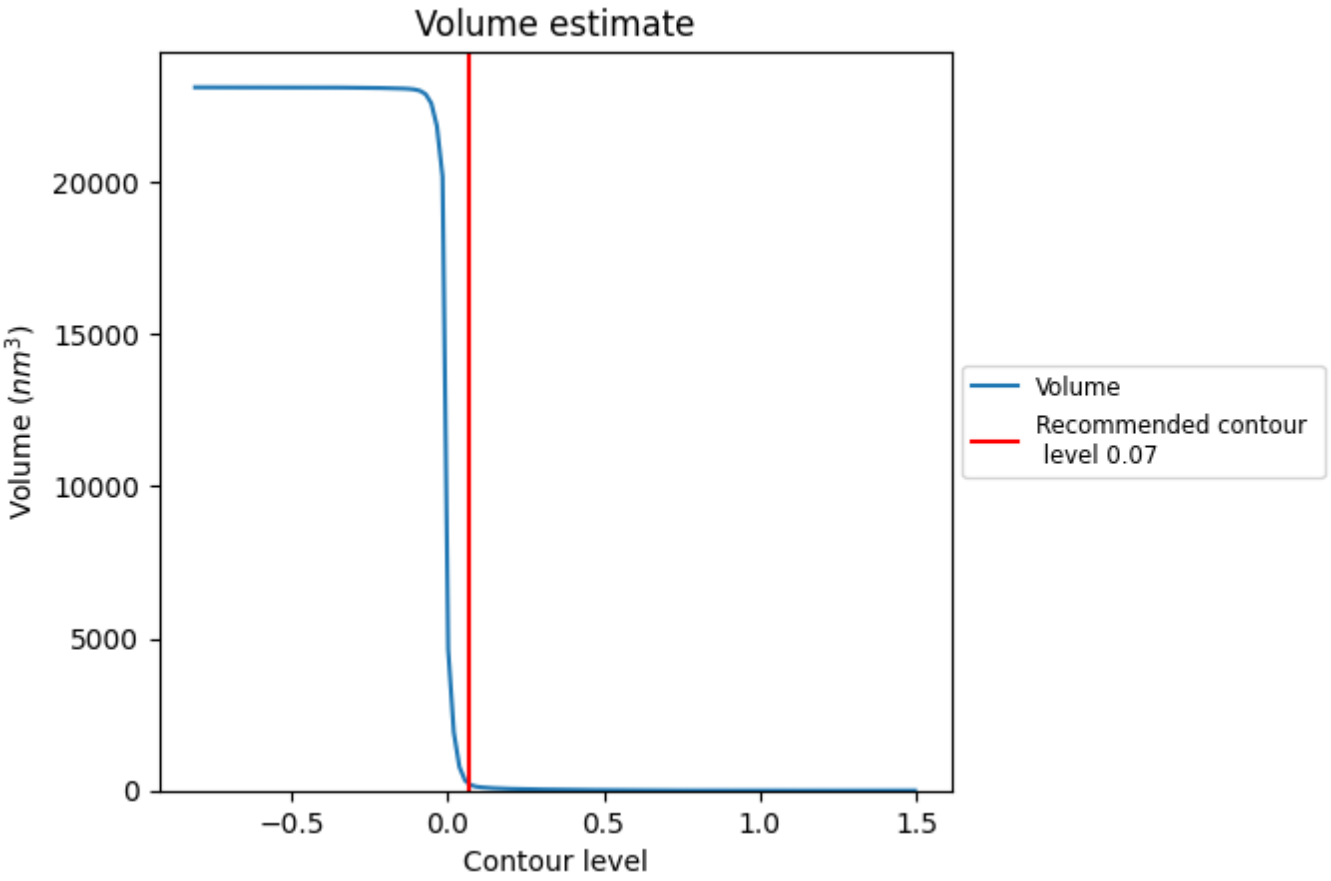
This section contains the results of statistical analysis of the map.

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.

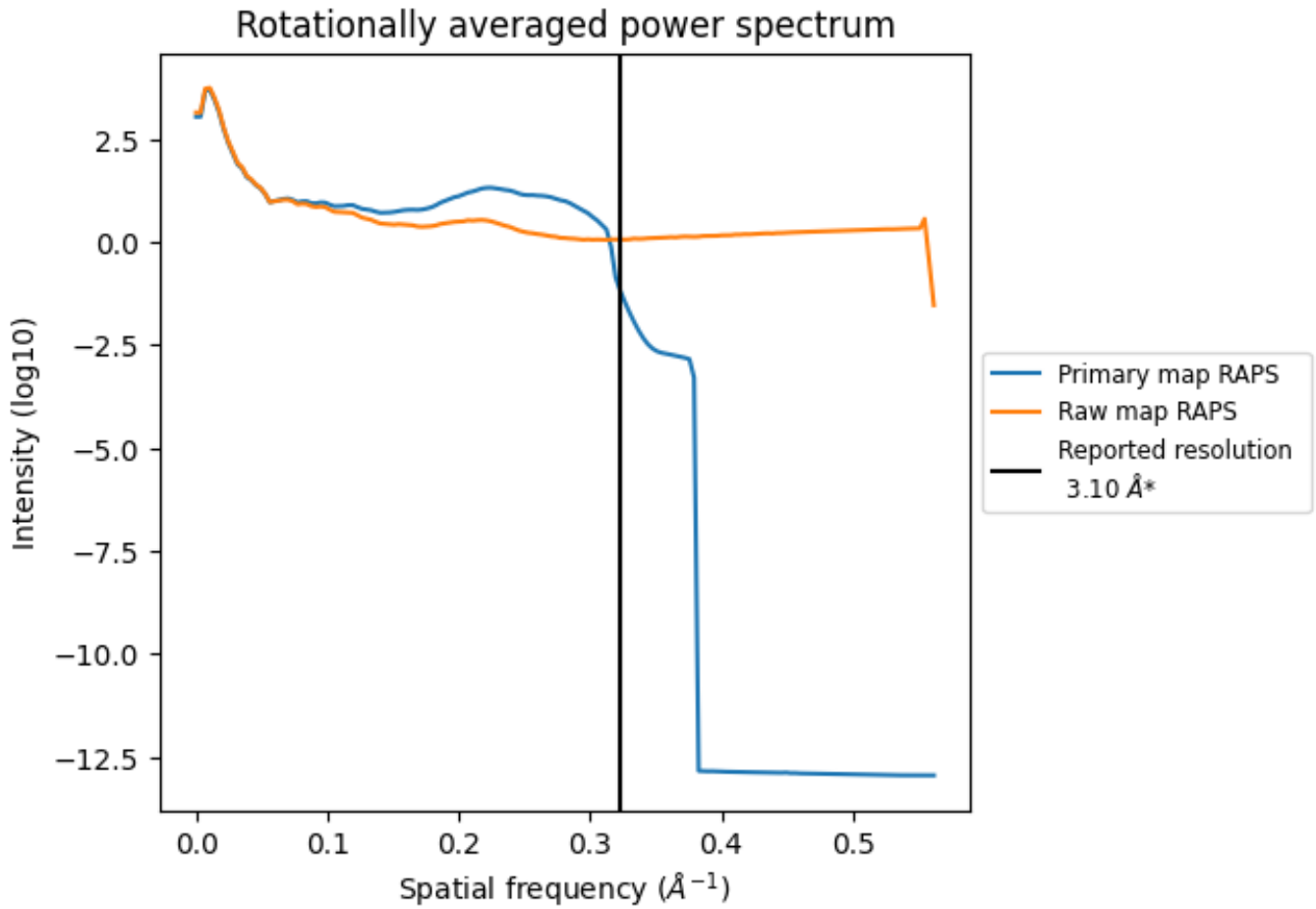
7.2 Volume estimate



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 201 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)

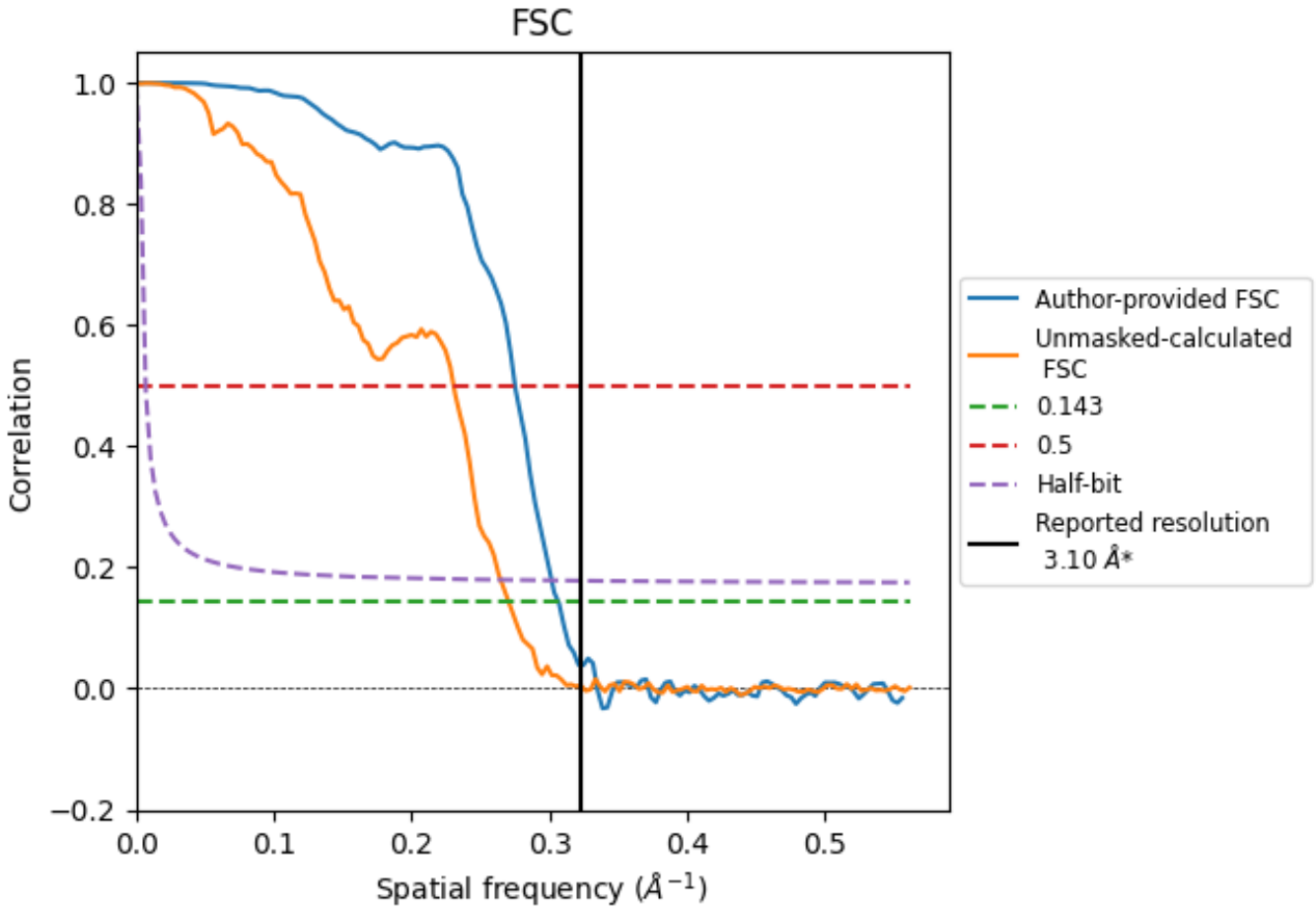


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.26	3.63	3.31
Unmasked-calculated*	3.70	4.33	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %

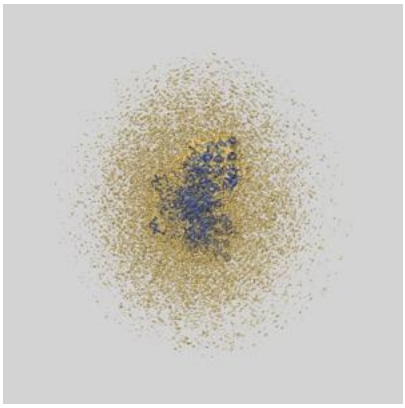
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-81083 and PDB model 27DN. Per-residue inclusion information can be found in section 3 on page 4.

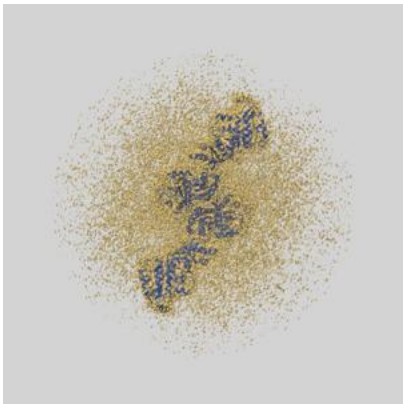
9.1 Map-model overlay



X



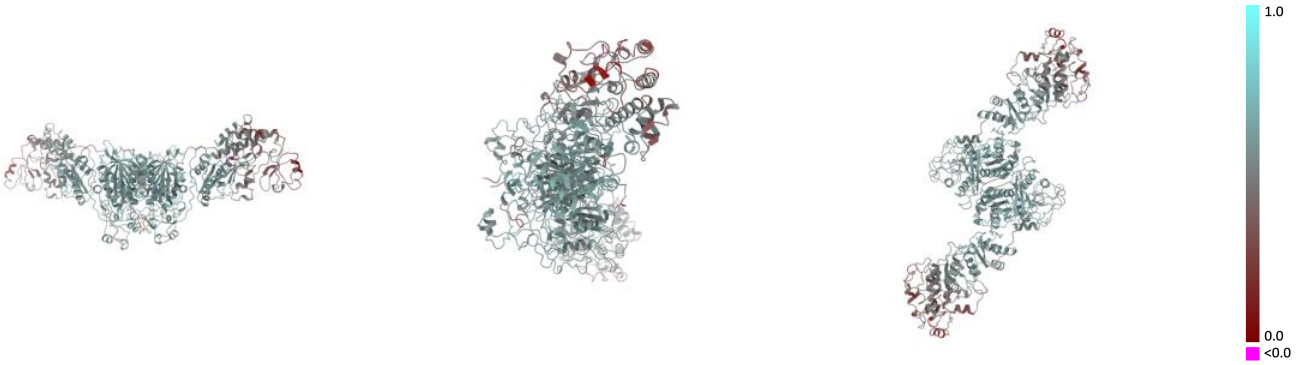
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

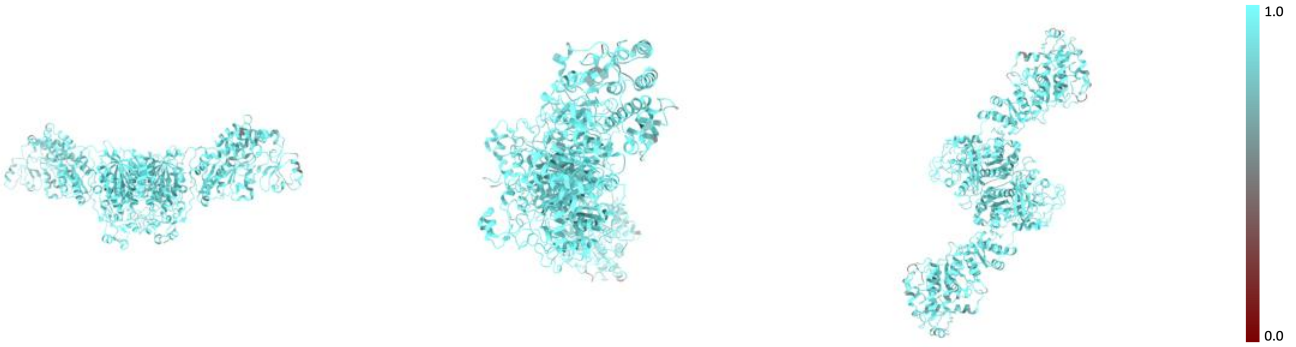
9.2 Q-score mapped to coordinate model (i)



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.

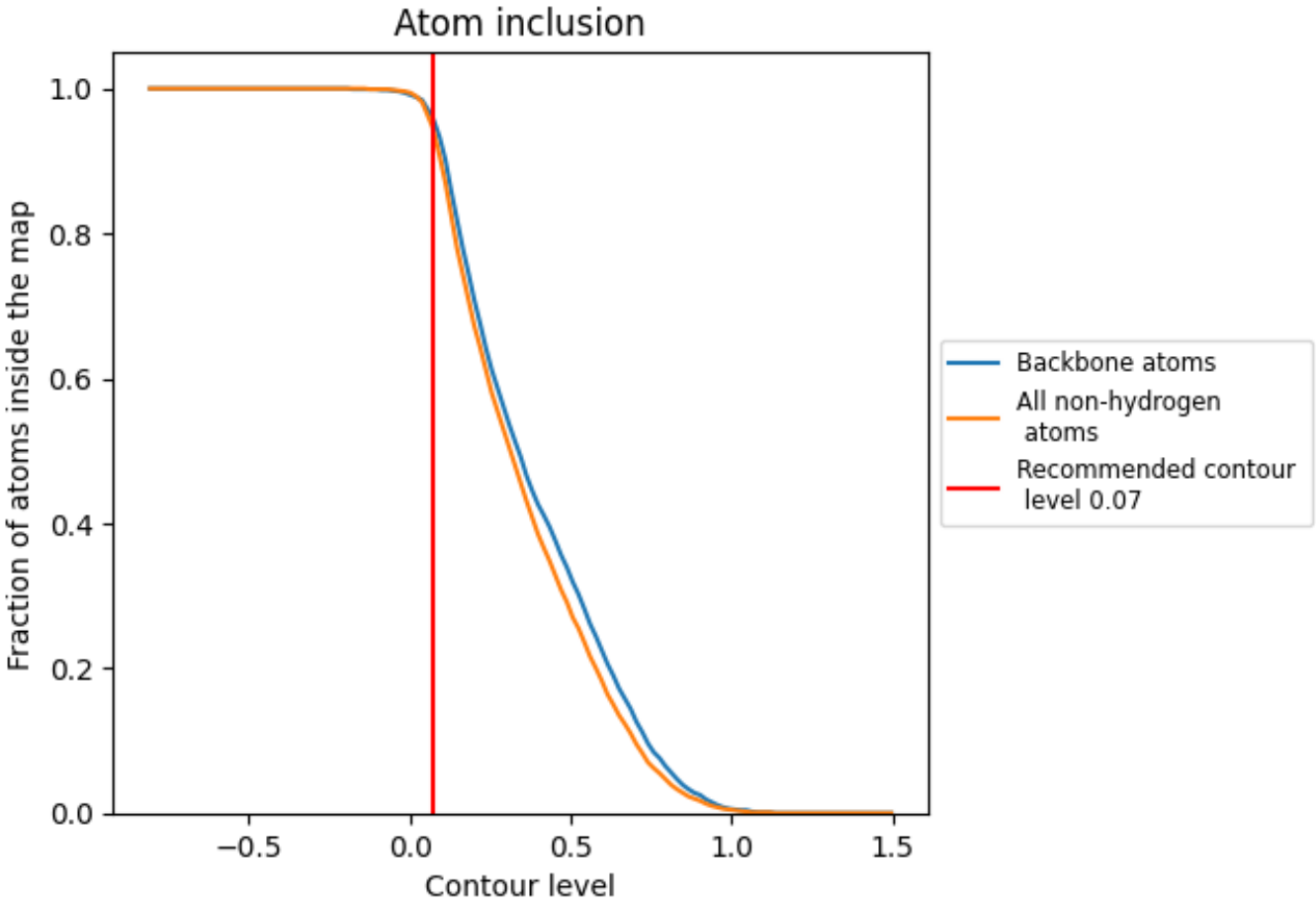
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.07) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9480	0.5280
A	0.9500	0.5290
B	0.9470	0.5270