wwPDB EM Validation Summary Report

Feb 22, 2025 – 04:04 PM EST

PDB ID	:	9BDE
EMDB ID	:	EMD-44450
Title	:	Middle Region of Apolipoprotein B 100 bound to Low Density Lipoprotein Receptor
Authors	:	Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on	:	2024-04-11
Resolution	:	4.18 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:

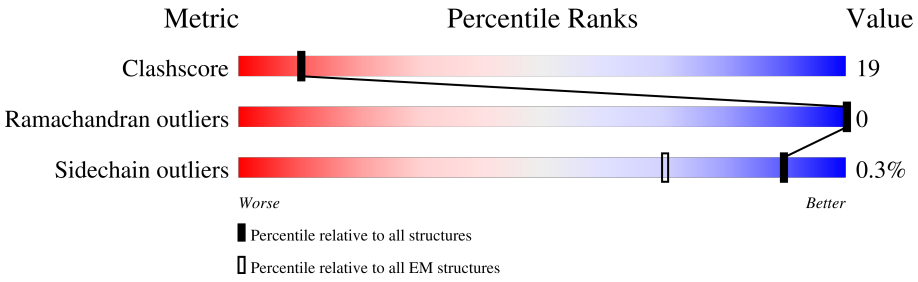
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 4.18 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	H	234	45% 31% 24%
2	A	4563	5% 15% 9% 75%
3	L	219	57% 25% 18%
4	B	545	55% 30% 14%
5	N	131	66% 28% 5%
6	R	860	6% 19% 13% 68%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17216 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 Legobody 8D3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	177	Total	C	N	O	S	0	0
			1289	818	213	250	8		

- Molecule 2 is a protein called Apolipoprotein B 100.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1121	Total	C	N	O	S	0	0
			8453	5327	1437	1677	12		

- Molecule 3 is a protein called Legobody 8D3 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	180	Total	C	N	O	S	0	0
			1244	780	201	258	5		

- Molecule 4 is a protein called Maltose/maltodextrin-binding periplasmic protein,Immunoglobulin G-binding protein A,Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	466	Total	C	N	O	S	0	0
			3396	2161	545	686	4		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0AEX9
B	361	ALA	GLN	conflict	UNP P02976
B	362	LEU	ASN	conflict	UNP P02976
B	365	ALA	TYR	conflict	UNP P02976
B	366	GLN	GLU	conflict	UNP P02976
B	369	ILE	HIS	conflict	UNP P02976
B	370	MET	LEU	conflict	UNP P02976
B	404	GLU	ASP	conflict	UNP P02976

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	405	HIS	ALA	conflict	UNP P02976
B	410	GLY	-	linker	UNP P02976
B	411	GLY	-	linker	UNP P02976
B	412	SER	-	linker	UNP P02976
B	413	GLY	-	linker	UNP P02976
B	414	GLY	-	linker	UNP P02976
B	415	ALA	-	linker	UNP P02976
B	416	GLY	-	linker	UNP P02976
B	417	SER	-	linker	UNP P02976
B	418	GLY	-	linker	UNP P02976
B	468	GLY	-	linker	UNP P02976
B	469	GLY	-	linker	UNP P02976
B	470	GLY	-	linker	UNP P02976
B	471	SER	-	linker	UNP P02976
B	472	GLY	-	linker	UNP P02976
B	473	GLY	-	linker	UNP P02976
B	474	GLY	-	linker	UNP P02976
B	475	SER	-	linker	UNP P02976
B	476	GLY	-	linker	UNP P02976
B	477	GLY	-	linker	UNP P02976
B	478	SER	-	linker	UNP P02976
B	537	GLY	-	expression tag	UNP P19909
B	538	SER	-	expression tag	UNP P19909
B	539	GLY	-	expression tag	UNP P19909
B	540	HIS	-	expression tag	UNP P19909
B	541	HIS	-	expression tag	UNP P19909
B	542	HIS	-	expression tag	UNP P19909
B	543	HIS	-	expression tag	UNP P19909
B	544	HIS	-	expression tag	UNP P19909
B	545	HIS	-	expression tag	UNP P19909

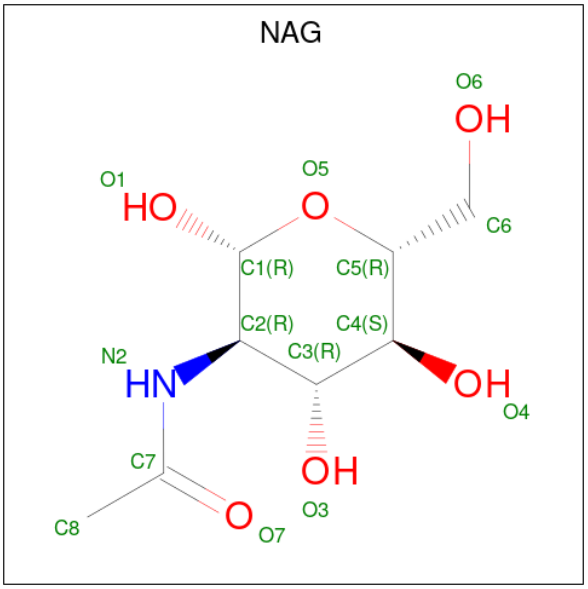
- Molecule 5 is a protein called ApoB100 nanobody 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	124	Total	C	N	O	S	0	0
			859	538	153	164	4		

- Molecule 6 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	272	Total	C	N	O	S	0	0
			1898	1125	322	407	44		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

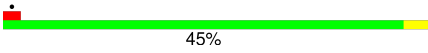
Mol	Chain	Residues	Atoms		AltConf
8	R	7	Total	Ca	0
			7	7	

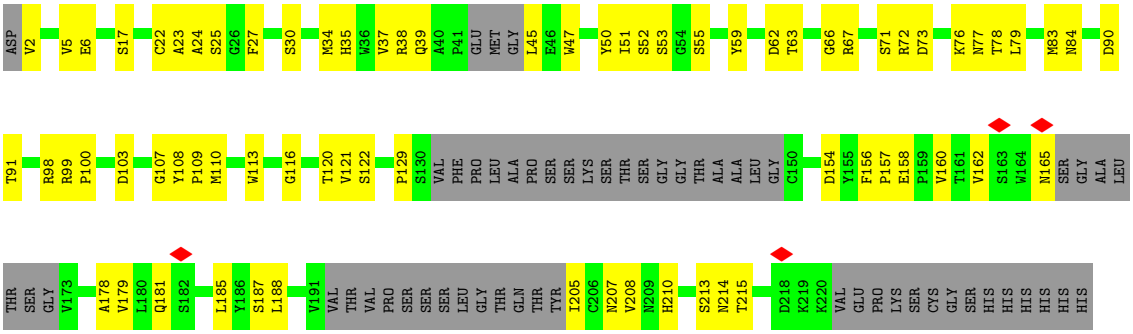
3 Residue-property plots (i)

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: Legobody 8D3 Fab Heavy Chain

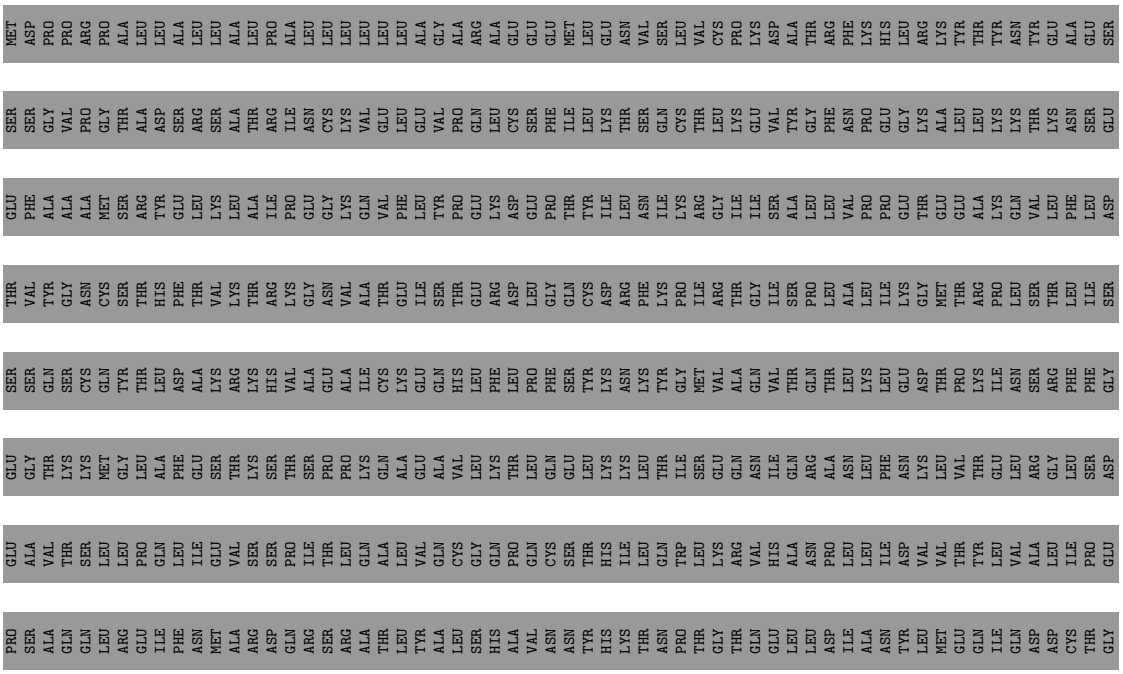
Chain H:





• Molecule 2: Apolipoprotein B 100

Chain A:



ASP GLU ASP TYR THR TYR LEU ILE LEU ARG VAL ILE GLY ASN MET GLY GLN THR MET GLU GLN LEU THR PRO GLU LEU LYS SER SER ILE LEU LYS CYS VAL GLN SER THR LYS PRO SER LEU MET ILE GLN LYS ALA ALA ILE GLN ALA LEU ARG LYS MET GLU PRO LYS ASP LYS ASP

GLN GLU VAL LEU LEU GLN THR PHE LEU ASP ASP ALA SER PRO GLY ASP LYS ARG LEU ALA ALA TYR LEU MET LEU MET ARG SER PRO SER GLN ALA ASP ILE ASN LYS ILE VAL GLN ILE LEU PRO TRP GLU GLN ASN GLU GLN VAL LYS ASN PHE VAL ALA SER HIS ILE ALA ASN ILE

LEU ASN SER GLU GLU LEU ASP ILE GLN ASP LEU LYS LYS LEU VAL LYS GLU ALA LEU LYS GLU SER GLN LEU PRO THR VAL MET ASP PHE ARG LYS PHE SER ARG ASN TYR GLN LEU TYR LYS SER VAL SER LEU PRO SER LEU ASP PRO ALA SER ALA LYS ILE GLU GLY ASN LEU ILE

PHE ASP PRO ASN ASN TYR LEU PRO LYS GLU SER MET LEU LYS THR THR LEU THR ALA PHE GLY PHE ALA SER ALA ASP LEU ILE GLU ILE GLY LEU GLU GLY LYS GLY PHE GLU PRO THR LEU GLU ALA LEU PHE GLY LYS GLN GLY PHE PHE PRO ASP SER VAL ASN LYS ALA LEU TYR

TRP VAL ASN GLY GLN VAL PRO ASP GLY VAL SER LYS VAL LEU VAL ASP HIS PHE GLY TYR THR LYS ASP ASP LYS HIS GLU GLN ASP MET VAL ASN GLY ILE MET LEU SER VAL GLU LYS LEU ILE LYS ASP LEU LYS SER LYS GLU VAL PRO GLU ALA ARG ALA TYR LEU ARG ILE LEU

GLY GLU GLU LEU GLY PHE ALA SER LEU HIS ASP LEU GLN LEU LEU GLY LYS LEU LEU LEU MET GLY ALA ARG THR LEU GLN GLY ILE PRO GLN MET ILE GLY GLU VAL ILE ARG LYS GLY SER LYS ASN ASP PHE PHE LEU HIS TYR ILE PHE MET GLU ASN ALA PHE GLU LEU PRO THR

GLY ALA GLY LEU GLN LEU GLN ILE SER SER SER GLY VAL ILE ALA PRO GLY ALA LYS ALA GLY VAL LYS LEU GLU VAL ALA ASN MET GLN ALA GLU LEU VAL ALA LYS PRO SER VAL SER VAL GLU PHE VAL THR ASN MET GLY ILE ILE ILE PRO ASP PHE ALA ARG SER GLY VAL GLN

MET ASN THR ASN PHE PHE HIS GLU SER GLY LEU GLU ALA HIS VAL ALA LEU LYS ALA GLY LYS LEU LYS PHE ILE ILE PRO SER PRO LYS ARG PRO VAL LYS LEU LEU SER GLY GLY ASN THR LEU HIS LEU VAL SER THR THR LYS THR GLU VAL ILE PRO PRO LEU ILE GLU ASN ARG

GLN SER TRP SER VAL CYS LYS GLN VAL PHE PRO GLY LEU ASN TYR CYS THR SER GLY ALA TYR SER ASN ALA SER SER THR ASP SER ALA SER TYR TYR PRO LEU THR GLY ASP THR ARG LEU GLU LEU GLU LEU ARG PRO THR GLY GLU ILE GLU GLN TYR SER VAL SER ALA THR TYR

GLU LEU GLN ARG GLU ASP ARG ALA LEU VAL ASP THR LEU LYS PHE VAL THR GLN ALA GLU GLY ALA LYS GLN THR GLU ALA THR MET THR PHE LYS TYR ASN ARG GLN SER MET THR LEU SER SER GLU VAL GLN ILE PRO ASP PHE ASP VAL ASP LEU GLY THR ILE LEU ARG VAL ASN

ASP GLU SER THR GLU GLY LYS THR SER TYR ARG LEU THR LEU ASP ILE GLN ASN LYS LYS ILE THR GLU VAL ALA LEU MET GLY HIS LEU SER CYS ASP THR LYS GLU GLU ARG LYS ILE LYS GLY VAL ILE SER ILE PRO ARG LEU GLN ALA GLU ALA ARG SER GLU ILE LEU ALA HIS

TRP SER PRO ALA LYS LEU LEU LEU GLN MET ASP SER SER ALA THR ALA TYR GLY SER THR VAL SER LYS ARG VAL ALA TRP HIS TYR ASP GLU GLU LYS ILE GLU PHE GLU TRP ASN THR GLY THR ASN VAL ASP THR LYS LYS MET THR SER ASN PHE PRO VAL ASP LEU SER ASP TYR

PRO LYS SER LEU HIS MET TYR ALA ASN ARG LEU LEU ASP HIS ARG VAL PRO GLN THR ASP MET THR PHE ARG HIS VAL GLY SER LYS LEU ILE VAL ALA MET SER SER TRP LEU GLN LYS ALA SER GLY SER LEU PRO TYR THR GLN THR LEU GLN ASP HIS LEU ASN SER LEU LYS GLU

PHE ASN LEU GLN ASN MET GLY LEU PRO ASP PHE HIS ILE PRO GLU ASN LEU PHE LEU LYS SER ASP GLY ARG VAL LYS TYR THR LEU ASN LYS ASN SER LEU LYS ILE GLU ILE PRO LEU PRO PHE GLY GLY LYS SER SER ARG ASP LEU LYS MET LEU GLU THR VAL ARG THR PRO ALA

LEU HIS PHE LYS SER VAL GLY PHE HIS LEU PRO SER ARG GLU PHE GLN VAL PRO THR PHE THR ILE PRO LYS LEU TYR GLN LEU GLN VAL PRO LEU LEU GLY VAL LEU ASP LEU SER THR ASN VAL TYR SER ASN LEU TYR ASN TRP SER ALA SER TYR SER GLY GLY ASN THR SER THR

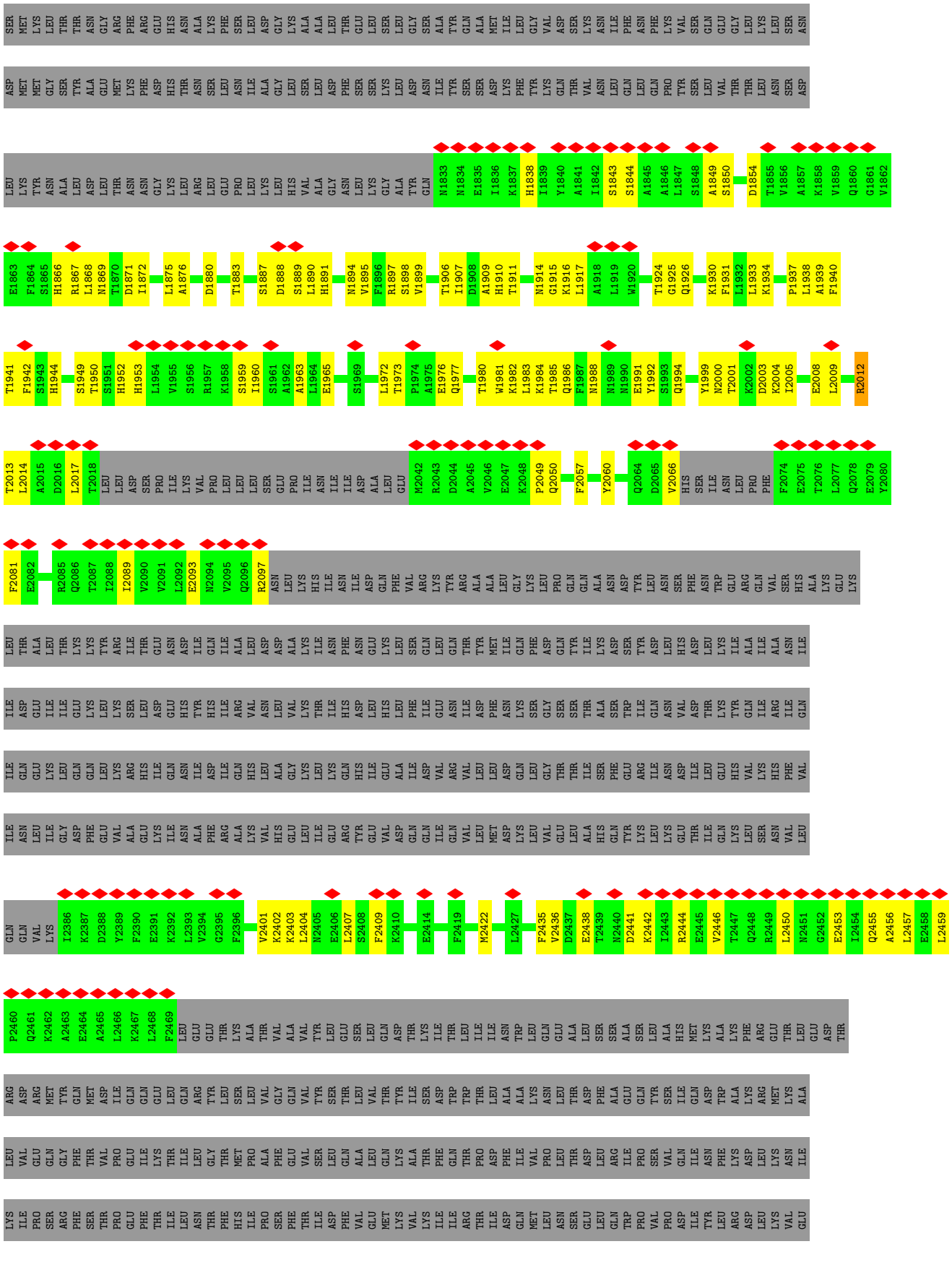
ASP HIS PHE SER LEU ARG ALA ARG TYR HIS MET LYS ALA ASP SER VAL VAL ASP LEU LEU SER TYR ASN VAL GLN GLY SER GLY GLU THR THR TYR ASP HIS LYS ASN THR PHE THR LEU SER CYS ASP GLY SER LEU ARG HIS LYS PHE LEU ASP SER ASN ILE LYS PHE SER HIS VAL

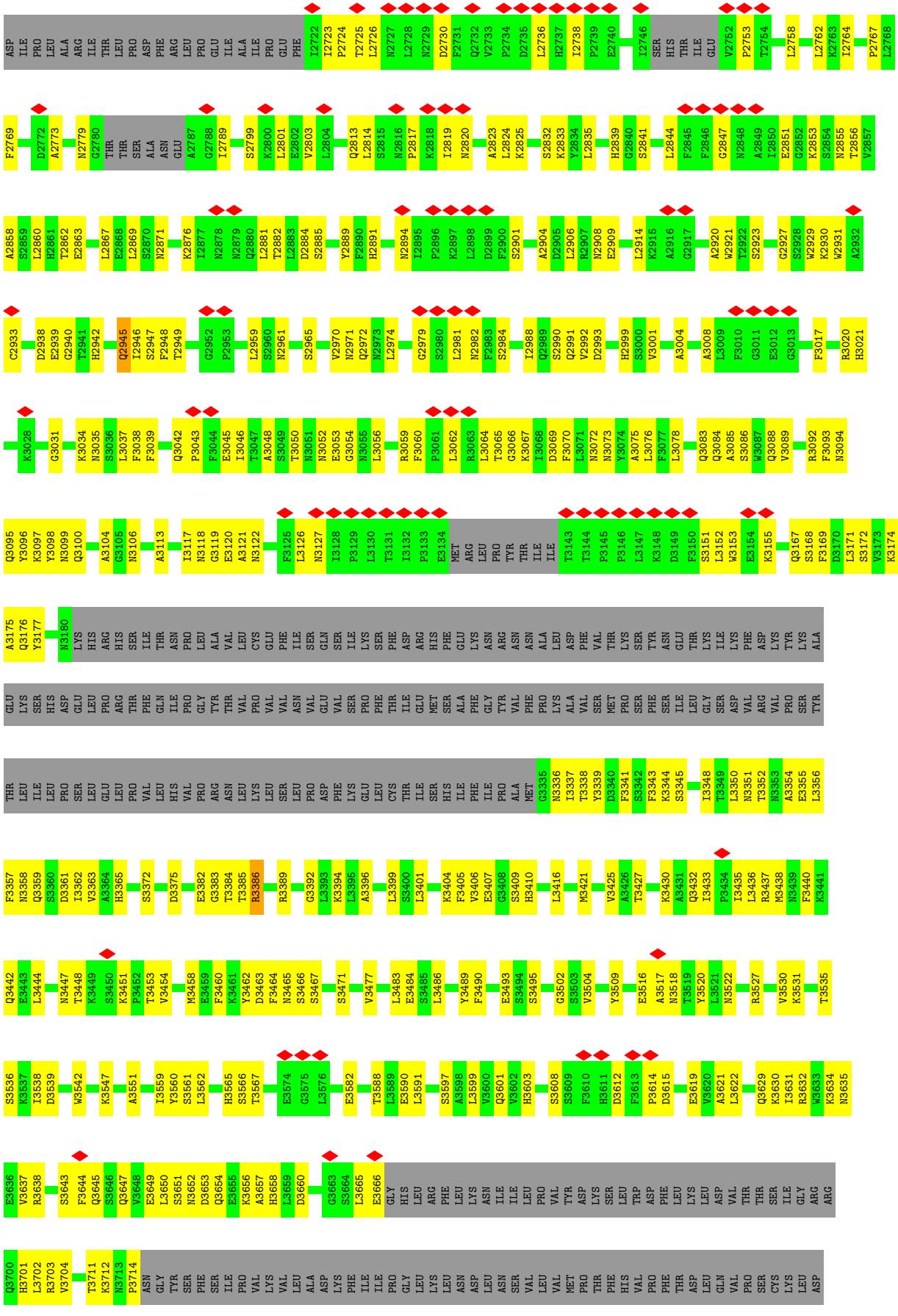
GLU LYS LEU GLY ASN ASN PRO VAL SER LYS GLY LEU LEU ILE PHE ASP ALA SER SER SER TRP GLY PRO GLN MET SER ALA SER VAL HIS LEU ASP SER LYS LYS LYS GLN HIS LEU PHE VAL LYS GLU VAL LYS ILE ASP GLY GLN PHE ARG VAL SER SER PHE TYR ALA LYS GLY THR

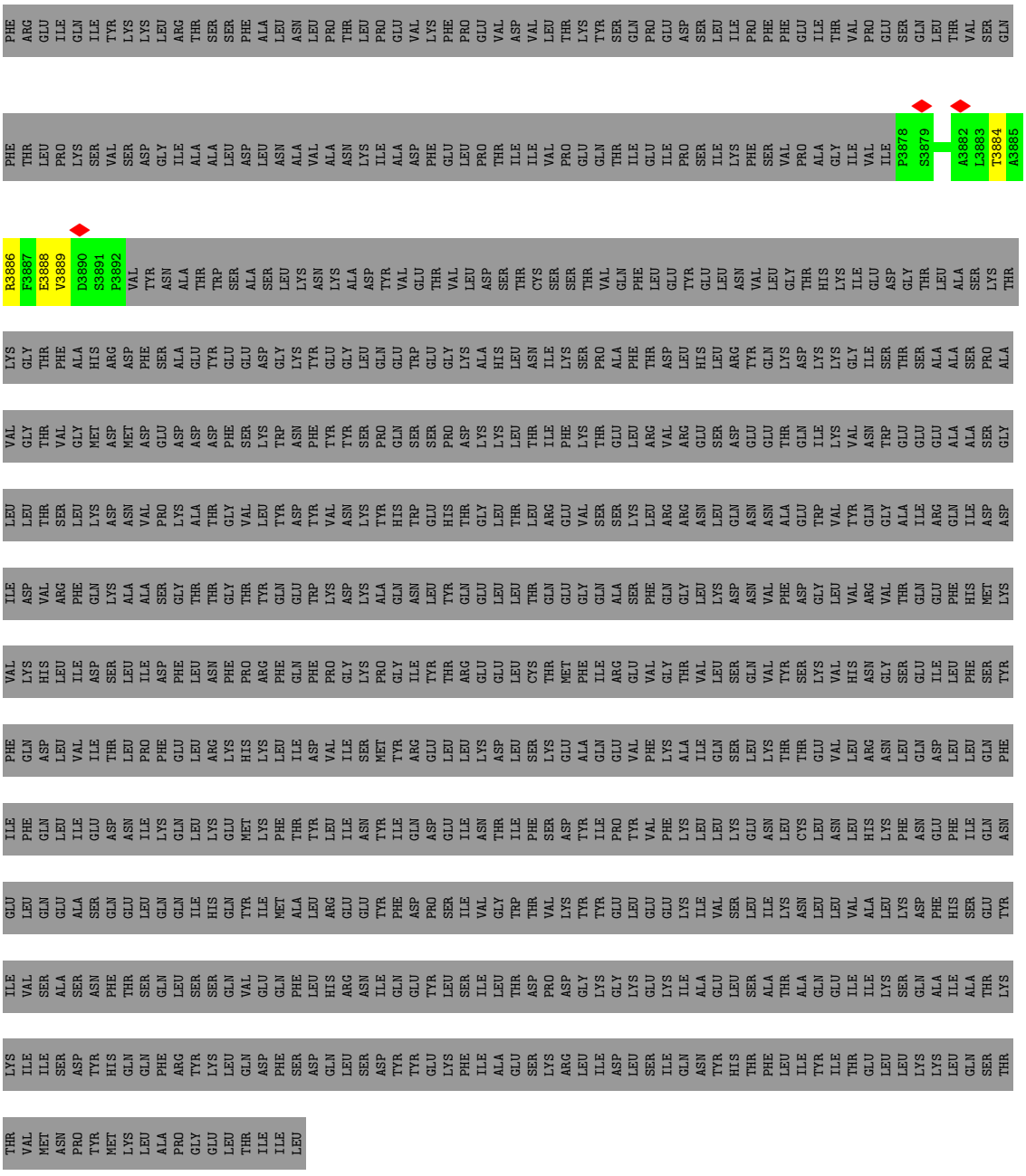
TYR GLY LEU SER CYS GLN ARG ASP PRO ASN THR GLY ARG LEU ASN GLY GLU SER ASN LEU ARG PHE ASN SER SER TYR LEU GLN GLY THR ASN GLN ILE THR GLY ARG TYR GLU ASP GLY THR LEU SER LEU THR SER THR SER ASP LEU GLN SER GLY ILE ILE LYS ASN THR ALA SER

LEU LYS TYR GLU ASN TYR GLU LEU THR LEU LYS SER ASP THR ASN GLY LYS TYR LYS ASN PHE ALA THR SER ASN LYS MET ASP MET THR PHE SER LYS GLN ASN ALA LEU LEU ARG SER GLU TYR GLN ALA ASP TYR GLU SER LEU ARG PHE PHE SER LEU LEU SER GLY SER LEU ASN

SER HIS GLY LEU GLU LEU ASN ALA ASP ILE LEU GLY THR ASP LYS ILE ASN SER GLY ALA HIS LYS ALA THR LEU ARG ILE GLY GLN ASP GLY ILE SER THR SER ALA THR THR ASN LEU LYS CYS SER LEU LEU VAL LEU GLU ASN GLU LEU ASN ALA GLU LEU GLY LEU SER GLY ALA

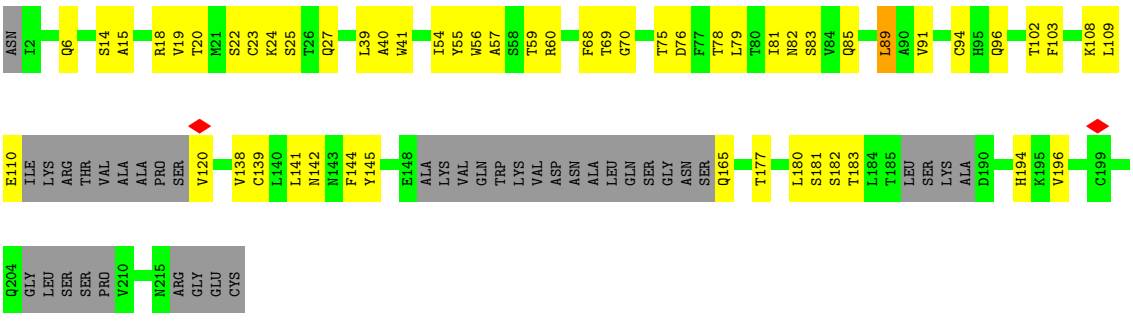

SER MET LYS LEU THR THR ASN GLY ARG PHE ARG GLU HIS ASN ALA LYS PHE SER LEU ASP GLY LYS ALA ALA LEU THR GLU LEU SER LEU GLY SER ALA TYR GLN ALA MET ILE LEU GLY VAL ASP SER LYS ASN ILE PHE ASN PHE LYS VAL SER GLN GLU GLY LEU LYS LEU SER ASN
ASP MET MET GLY SER TYR ALA GLU MET LYS PHE ASP HIS THR ASN SER LEU ASN ILE ALA GLY LEU SER SER LYS LEU ASP ASN ILE TYR SER SER ASP LYS PHE TYR LYS GLN THR VAL ASN LEU GLN LEU GLN PRO TYR SER LEU VAL THR THR LEU ASN SER ASP
LEU LYS TYR ASN ALA LEU ASP LEU THR ASN ASN GLY LYS LEU ARG LEU GLU PRO LEU LYS LEU HIS VAL ALA GLY ASN LEU LYS GLY ALA TYR GLN N1833 N1834 E1835 I1836 K1837 H1838 I1839 Y1840 A1841 I1842 S1843 S1844 A1845 A1846 L1847 S1848 A1849 S1850 D1854 T1855 V1856 A1857 K1858 V1859 Q1860 G1861 V1862
E1863 F1864 S1865 H1866 R1867 L1868 N1869 T1870 D1871 I1872 L1875 A1876 D1880 T1883 S1887 D1888 S1889 L1890 H1891 N1894 V1895 F1896 R1897 S1898 V1899 T1906 I1907 D1908 A1909 H1910 T1911 N1914 G1915 K1916 L1917 A1918 L1919 W1920 T1924 G1925 Q1926 K1930 F1931 L1932 L1933 K1934 P1937 L1938 A1939 F1940
T1941 F1942 S1943 H1944 S1949 T1950 S1951 H1952 H1953 L1954 V1955 S1956 R1957 K1958 S1959 I1960 S1961 A1962 A1963 L1964 E1965 S1969 L1972 T1973 P1974 A1975 E1976 Q1977 T1980 W1981 K1982 L1983 K1984 T1985 Q1986 F1987 N1988 N1989 N1990 E1991 Y1992 S1993 Q1994 Y1999 N2000 T2001 K2002 D2003 K2004 I2005 E2008 L2009 R2012
T2013 L2014 A2015 D2016 L2017 T2018 LEU LEU ASP SER PRO ILE LYS VAL PRO LEU LEU LEU SER GLU PRO ILE ASN ILE ILE ASP ALA LEU GLU M2042 R2043 D2044 A2045 V2046 E2047 K2048 P2049 Q2050 F2057 Y2060 Q2064 D2065 V2066 HIS SER ILE ASN LEU PRO PHE F2074 E2075 T2076 L2077 Q2078 E2079 Y2080
F2081 E2082 R2085 Q2086 T2087 I2088 T2089 V2090 V2091 L2092 E2093 N2094 V2095 Q2096 R2097 ASN LEU LYS HIS ILE ASN ILE ASP GLN PHE VAL ARG LYS TYR ARG ALA ALA LEU GLY LYS LEU PRO GLN GLN ALA ASN ASP TYR LEU ASN SER PHE ASN TRP GLU ARG GLN VAL SER HIS ALA LYS GLU LYS
LEU THR ALA LEU THR LYS LYS TYR ARG ILE THR GLU ASN ASP ILE GLN ILE ALA LEU ASP ASP ALA LYS ILE ASN PHE ASN GLU LYS LEU SER GLN LEU GLN THR TYR MET ILE GLN PHE ASP GLN TYR ILE LYS ASP SER TYR ASP LEU HIS ASP LEU LEU LYS ILE ALA ILE ALA ASN ILE
ILE ASP GLU ILE ILE GLU LYS LEU LYS SER LEU ASP GLU HIS TYR HIS ILE ARG VAL ASN LEU VAL LYS THR ILE HIS ASP LEU HIS LEU PHE ILE GLU ASN ILE ASP PHE ASN LYS SER GLY SER SER THR ALA SER TRP ILE GLN ASN VAL ASP THR LYS TYR GLN ILE ARG ILE GLN
ILE GLN GLU LYS LEU GLN GLN LEU LYS ARG HIS ILE GLN ASN ILE ASP ILE GLN HIS LEU ALA GLY LYS LEU LYS GLN HIS ILE GLU GLU ALA ILE ASP VAL ARG VAL LEU LEU ASP GLN LEU GLY THR THR ILE SER PHE GLU ARG ILE ASN ASP ILE LEU GLU HIS VAL LYS HIS PHE VAL
ILE ASN LEU ILE GLY ASP PHE GLU VAL ALA GLU LYS ILE ASN ALA PHE ARG ALA LYS VAL HIS GLU LEU ILE GLU ARG TYR GLU VAL ASP GLN GLN ILE GLN LEU VAL LEU MET ASP LYS LEU VAL GLU LEU ALA HIS GLN TYR LYS LEU LYS GLU THR ILE GLN LYS LEU SER ASN VAL LEU
GLN GLN VAL LYS I2386 K2387 D2388 Y2389 F2390 E2391 K2392 L2393 V2394 G2395 F2396 V2401 K2402 K2403 L2404 N2405 E2406 L2407 S2408 F2409 K2410 E2414 F2419 M2422 L2427 F2435 V2436 D2437 E2438 T2439 N2440 D2441 K2442 I2443 R2444 E2445 V2446 T2447 Q2448 R2449 L2450 N2451 G2452 E2453 I2454 Q2455 A2456 L2457 E2458 L2459
P2460 Q2461 K2462 A2463 E2464 A2465 L2466 K2467 L2468 F2469 LEU GLU GLU THR LYS ALA THR VAL ALA VAL TYR LEU GLU SER LEU GLN ASP THR LYS ILE THR LEU ILE ILE ASN TRP LEU GLN GLU ALA LEU SER SER ALA GLU GLN LEU ALA HIS MET LYS ALA LYS PHE ARG GLU THR LEU GLU ASP THR
ARG ASP ARG MET TYR GLN MET ASP ILE GLN GLN GLU LEU GLN ARG TYR LEU SER LEU VAL GLY GLN VAL TYR SER THR LEU VAL THR TYR ILE SER ASP TRP TRP THR LEU ALA ALA LYS ASN LEU THR ASP PHE ALA GLU GLN TYR SER ILE GLN ASP TRP ALA LYS ARG MET LYS ALA
LEU VAL GLU GLN GLY PHE THR VAL PRO GLU ILE LYS THR ILE LEU LEU GLY THR MET PRO ALA PHE GLU VAL SER LEU GLN ALA LEU GLN LYS ALA THR PHE GLN THR PRO ASP PHE ILE VAL PRO LEU THR ASP LEU ARG ILE PRO SER VAL GLN ILE ASN PHE LYS ASP LEU ILE ASN
LYS ILE PRO SER ARG PHE SER PHE THR ILE ASP PHE VAL GLU MET LYS VAL LYS ILE ILE ARG THR PHE HIS ILE PRO SER PHE THR ILE ASP PHE VAL GLU MET LEU ASN SER GLU LEU GLN TRP PRO VAL PRO ASP ILE TYR LEU ARG ILE PRO SER VAL GLN ILE ASN PHE LYS ASP LEU ILE ASN





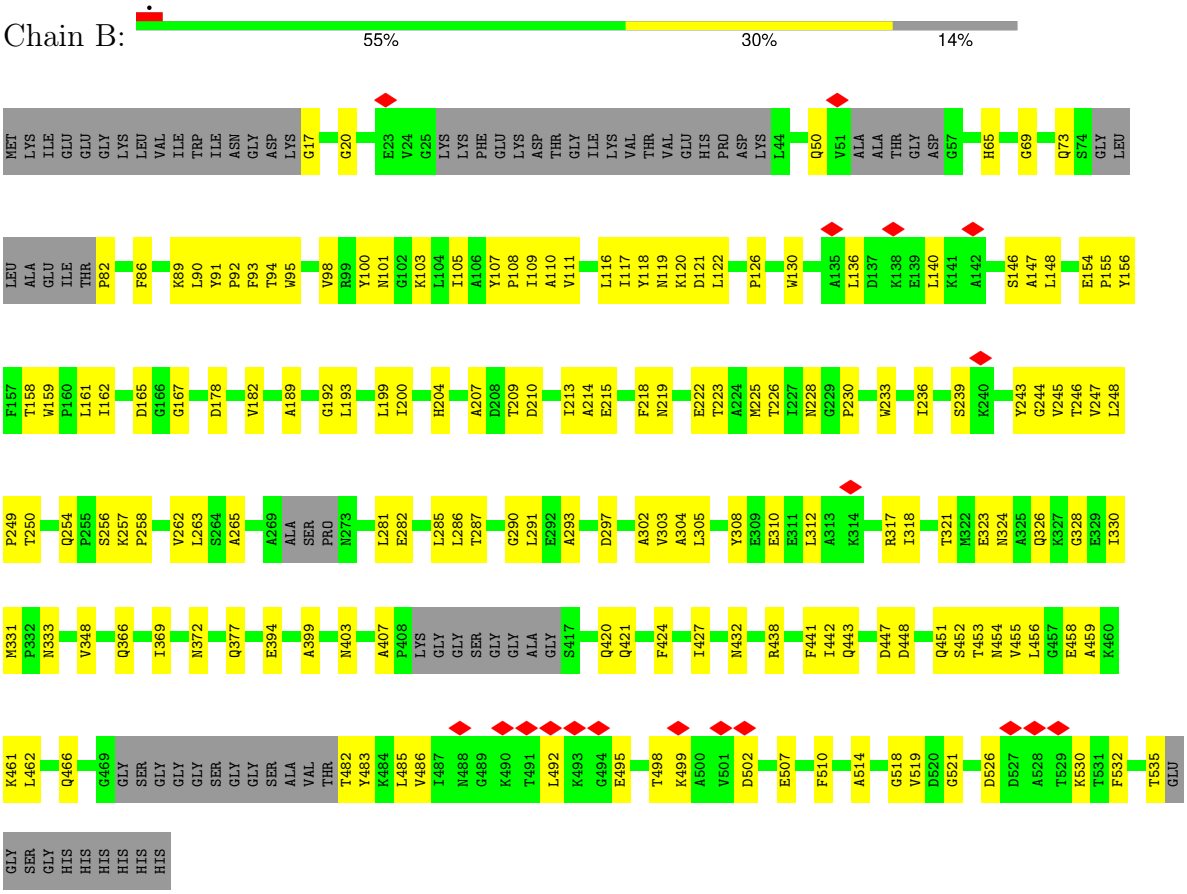
• Molecule 3: Legobody 8D3 Fab light chain

Chain L:



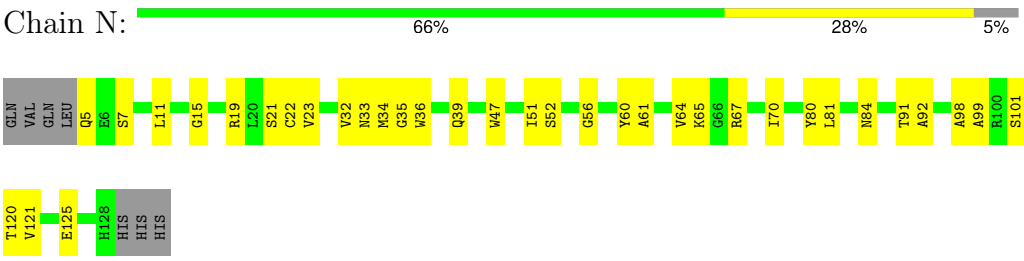
• Molecule 4: Maltose/maltodextrin-binding periplasmic protein,Immunoglobulin G-binding protein A,Immunoglobulin G-binding protein G

Chain B:



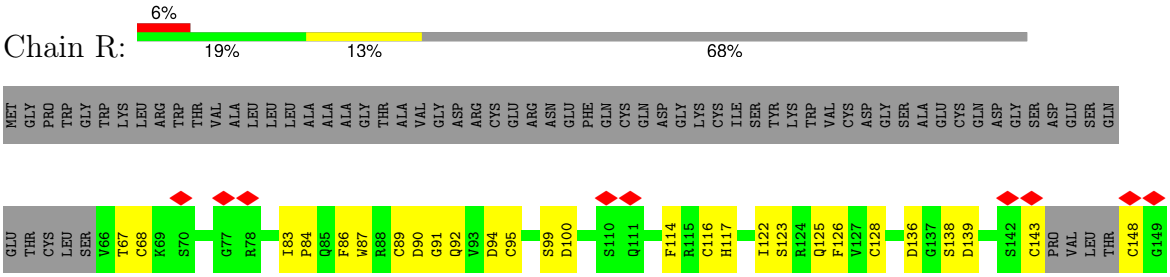
• Molecule 5: ApoB100 nanobody 4

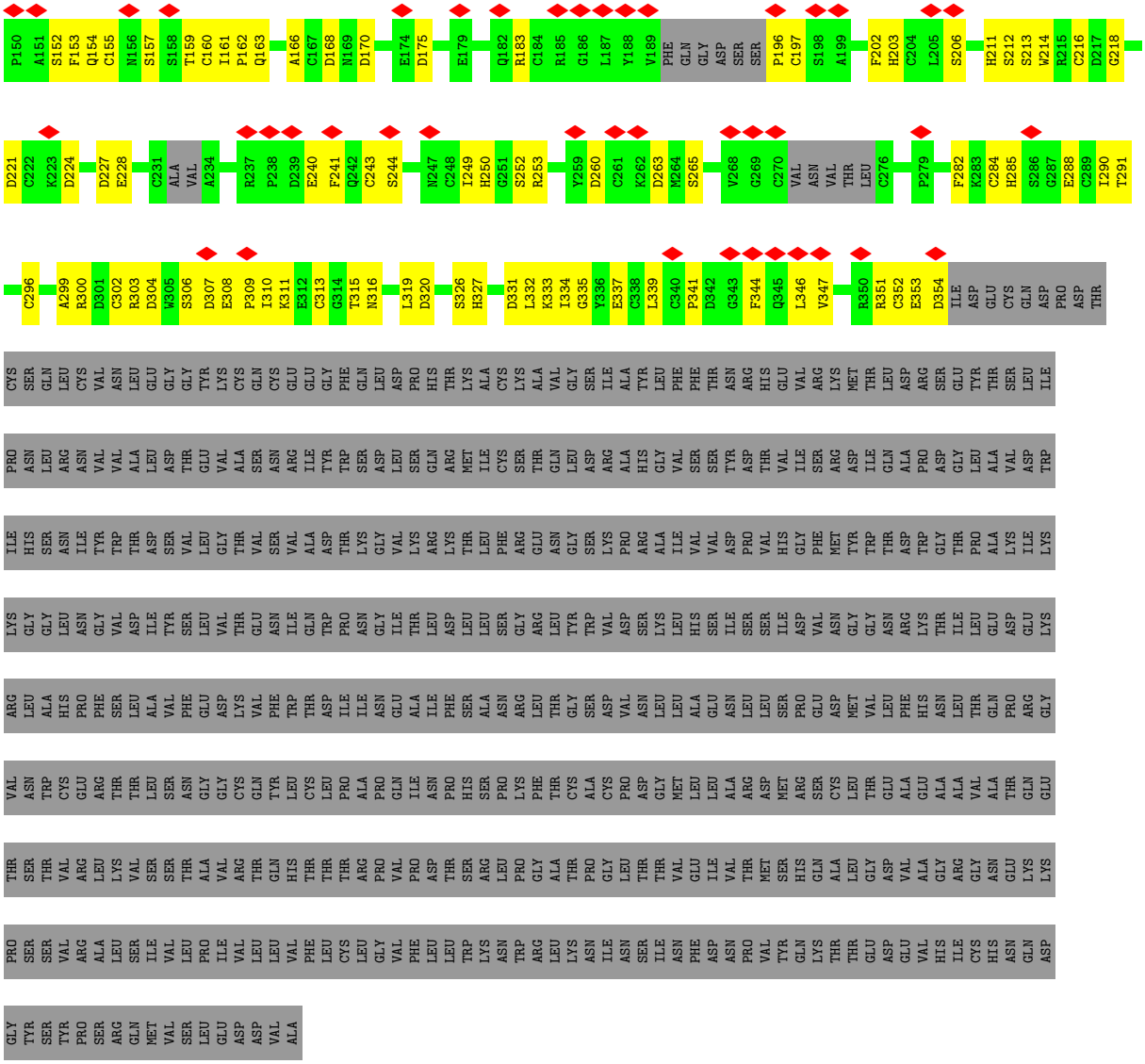
Chain N:



• Molecule 6: Low-density lipoprotein receptor

Chain R:




P150 A151 S152 F153 Q154 C155 N156 S157 S158 T159 C160 I161 P162 Q163 A166 C167 D168 N169 D170 E174 D175 E179 Q182 R183 C184 R185 G186 L187 Y188 V189 PHE GLN GLY ASP SER SER P196 C197 S198 A199 F202 H203 C204 L205 S206 H211 S212 S213 W214 R215 C216 D217 G218
D221 C222 K223 D224 D227 E228 C231 ALA VAL A234 R237 P238 D239 E240 F241 Q242 C243 S244 N247 C248 T249 H250 G251 S252 R253 Y259 D260 C261 K262 D263 M264 S265 V268 G269 C270 VAL ASN VAL THR LEU C276 P279 F282 K283 C284 H285 S286 G287 E288 C289 I290 T291
C296 A299 R300 D301 C302 R303 D304 W305 S306 D307 E308 P309 I310 K311 E312 C313 G314 T315 N316 L319 D320 S326 H327 D331 L332 K333 I334 G335 Y336 E337 C338 L339 C340 P341 D342 G343 F344 Q345 L346 V347 R350 R351 C352 E353 D354 ILE ASP GLU CYS GLN ASP PRO ASP THR
CYS SER GLN LEU CYS VAL ASN LEU GLU GLY GLY TYR LYS CYS GLN CYS GLU GLU GLY PHE GLN LEU ASP PRO HIS THR LYS ALA CYS LYS ALA VAL GLY SER ILE ALA TYR LEU PHE PHE THR ASN ARG HIS GLU VAL ARG LYS MET THR LEU ASP ARG SER GLU TYR THR SER LEU ILE
PRO ASN LEU ARG ASN VAL VAL ALA LEU ASP THR GLU VAL ALA SER ASN ARG ILE TYR TRP SER ASP LEU SER GLN ARG MET ILE CYS SER THR GLN LEU ASP ARG ALA HIS GLY VAL SER SER TYR ASP THR VAL ILE SER ARG ASP PRO ASP GLY LEU ALA VAL ASP TRP
ILE HIS SER ASN ILE TYR TRP THR ASP SER VAL LEU GLY THR VAL SER VAL ALA ASP THR LYS GLY VAL LYS ARG LYS THR LEU PHE ARG GLU ASN GLY SER LYS PRO ARG ALA ILE VAL VAL ASP PRO VAL HIS GLY PHE MET TYR TRP THR ASP TRP GLY THR PRO ALA LYS ILE LYS
LYS GLY GLY LEU ASN GLY VAL ASP ILE TYR SER LEU VAL THR GLU ASN ILE GLN TRP PRO ASN GLY VAL ILE THR LEU ASP LEU LEU SER GLY ARG LEU TYR TRP VAL ASP SER LYS LEU HIS SER ILE SER SER ILE ASP VAL ASN GLY GLY ASN ARG LYS THR ILE LEU GLU ASP GLU LYS
ARG LEU ALA HIS PRO PHE SER LEU ALA VAL PHE GLU ASP LYS VAL PHE TRP THR ASP ILE ILE ASN GLU ALA ILE PHE SER ALA ASN ARG LEU THR GLY SER ASP VAL ASN LEU LEU ALA GLU ASN LEU LEU SER PRO GLU ASP MET VAL LEU GLY ASN ARG GLN PRO ARG GLY
VAL ASN TRP CYS GLU ARG THR THR LEU SER ASN GLY GLY CYS GLN TYR LEU CYS LEU PRO ALA PRO GLN ILE ASN PRO HIS SER PRO LYS PHE THR CYS ALA CYS PRO ASP GLY MET LEU LEU ALA ARG ASP MET ARG SER CYS LEU THR GLU ALA GLU HIS ASN LEU THR GLN ALA GLU
THR SER THR VAL ARG LEU LYS VAL SER SER THR ALA VAL ARG THR GLN HIS THR THR PHE LEU CYS LEU PRO VAL ASP THR SER ARG LEU PRO GLY ALA THR PRO GLY LEU THR THR MET SER HIS GLN ALA LEU GLY ASP VAL ALA GLY ARG GLY ASN GLU LYS LYS
PRO SER SER VAL ARG ALA LEU SER ILE VAL LEU PRO ILE VAL LEU LEU VAL PHE LEU CYS LEU GLY VAL PHE LEU LEU TRP LYS ASN TRP ARG LEU LYS ASN ILE ASN SER ILE ASN PHE ASP ASN PRO VAL TYR GLN LYS THR THR GLU ASP VAL ALA GLU VAL HIS ILE CYS HIS ASN GLN ASP
GLY TYR SER TYR PRO SER ARG GLN MET VAL SER LEU GLU ASP ASP VAL ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527598	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 ($e^-/Å^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.494	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	Depositor

5 Model quality

5.1 Standard geometry

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

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	H	0.27	0/1320	0.50	0/1803
2	A	0.25	0/8603	0.50	0/11684
3	L	0.25	0/1267	0.53	1/1743 (0.1%)
4	B	0.25	0/3468	0.43	0/4753
5	N	0.28	0/877	0.53	0/1196
6	R	0.25	0/1932	0.50	0/2622
All	All	0.25	0/17467	0.49	1/23801 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	89	LEU	CA-CB-CG	5.25	127.38	115.30

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	H	1289	0	1173	55	0
2	A	8453	0	8047	300	0
3	L	1244	0	1077	38	0
4	B	3396	0	3063	132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	859	0	767	27	0
6	R	1898	0	1496	85	0
7	A	70	0	65	5	0
8	R	7	0	0	0	0
All	All	17216	0	15688	614	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 19.

The worst 5 of 614 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3565:HIS:HE2	2:A:3567:THR:HG1	1.20	0.88
2:A:3060:PHE:HB2	2:A:3064:LEU:HB2	1.64	0.77
2:A:2931:TRP:NE1	2:A:2933:CYS:SG	2.58	0.77
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.66	0.77
2:A:3017:PHE:HB3	2:A:3039:PHE:HB3	1.67	0.77

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	H	167/234 (71%)	160 (96%)	7 (4%)	0	100	100
2	A	1099/4563 (24%)	1019 (93%)	80 (7%)	0	100	100
3	L	170/219 (78%)	161 (95%)	9 (5%)	0	100	100
4	B	452/545 (83%)	438 (97%)	14 (3%)	0	100	100
5	N	122/131 (93%)	109 (89%)	13 (11%)	0	100	100
6	R	262/860 (30%)	232 (88%)	30 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2272/6552 (35%)	2119 (93%)	153 (7%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	135/199 (68%)	135 (100%)	0	100 100
2	A	902/4080 (22%)	897 (99%)	5 (1%)	84 88
3	L	124/192 (65%)	124 (100%)	0	100 100
4	B	323/433 (75%)	323 (100%)	0	100 100
5	N	75/103 (73%)	75 (100%)	0	100 100
6	R	202/755 (27%)	202 (100%)	0	100 100
All	All	1761/5762 (31%)	1756 (100%)	5 (0%)	90 92

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

Mol	Chain	Res	Type
2	A	1867	ARG
2	A	2012	ARG
2	A	2444	ARG
2	A	2945	GLN
2	A	3386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	3167	GLN
2	A	3635	ASN
4	B	119	ASN
4	B	420	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)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	4601	2	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
7	NAG	A	4603	2	14,14,15	0.74	0	17,19,21	2.31	3 (17%)
7	NAG	A	4604	2	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	A	4605	2	14,14,15	0.84	0	17,19,21	1.84	2 (11%)
7	NAG	A	4602	2	14,14,15	0.73	0	17,19,21	0.92	1 (5%)

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
7	NAG	A	4601	2	-	1/6/23/26	0/1/1/1
7	NAG	A	4603	2	-	4/6/23/26	0/1/1/1
7	NAG	A	4604	2	-	1/6/23/26	0/1/1/1
7	NAG	A	4605	2	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	4602	2	-	2/6/23/26	0/1/1/1

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})
7	A	4603	NAG	C2-N2-C7	8.23	133.94	122.90
7	A	4605	NAG	C1-O5-C5	6.44	120.82	112.19
7	A	4601	NAG	C2-N2-C7	3.05	126.99	122.90
7	A	4603	NAG	C8-C7-N2	2.62	120.47	116.12
7	A	4604	NAG	O5-C1-C2	-2.18	107.91	111.29

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4602	NAG	C8-C7-N2-C2
7	A	4602	NAG	O7-C7-N2-C2
7	A	4603	NAG	C8-C7-N2-C2
7	A	4603	NAG	O7-C7-N2-C2
7	A	4604	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4601	NAG	2	0
7	A	4604	NAG	1	0
7	A	4605	NAG	2	0

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.

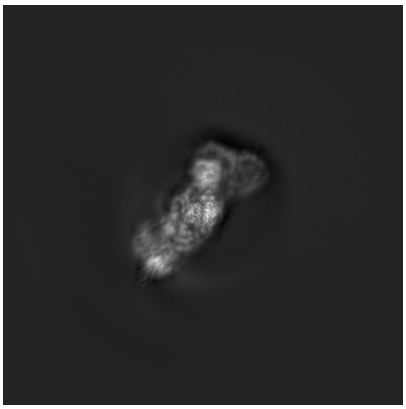
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44450. These allow visual inspection of the internal detail of the map and identification of artifacts.

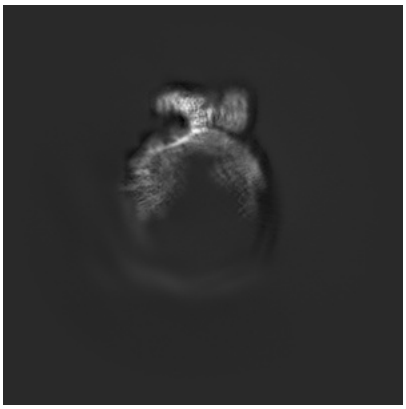
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

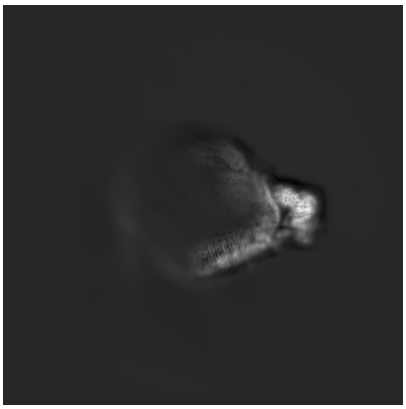
6.1.1 Primary map



X

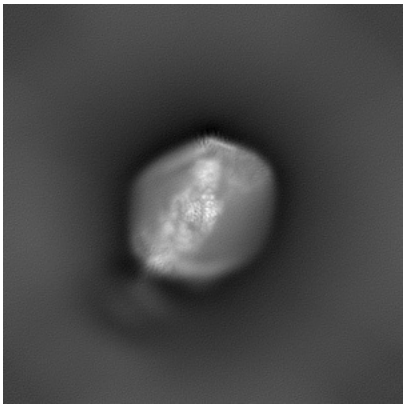


Y

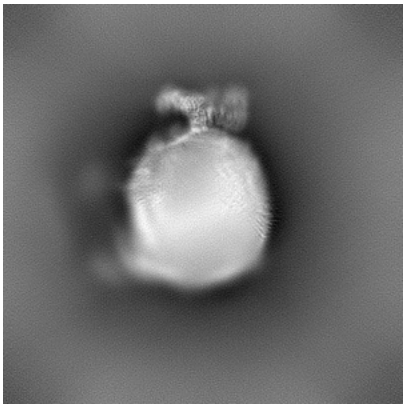


Z

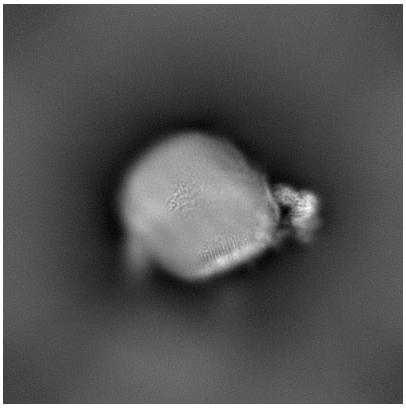
6.1.2 Raw map



X



Y



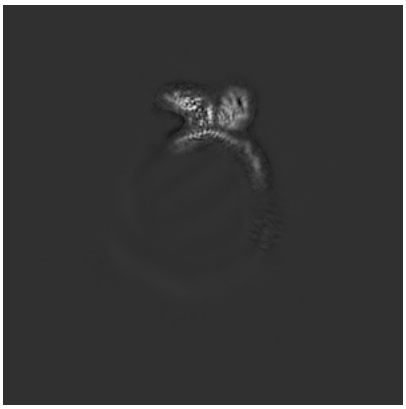
Z

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

6.2 Central slices (i)

6.2.1 Primary map

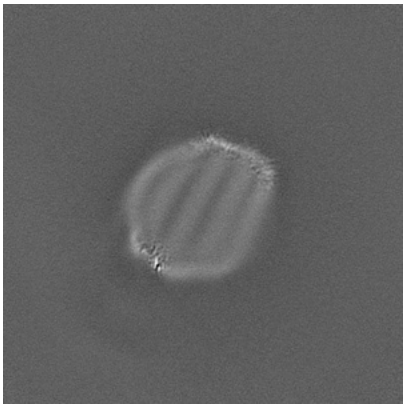
X Index: 168



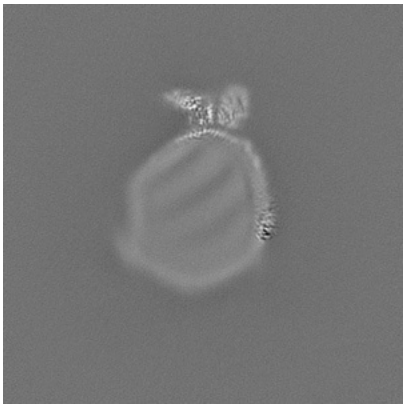
Y Index: 168

Z Index: 168

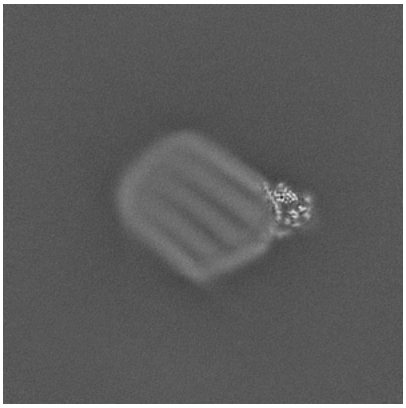
6.2.2 Raw map



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)

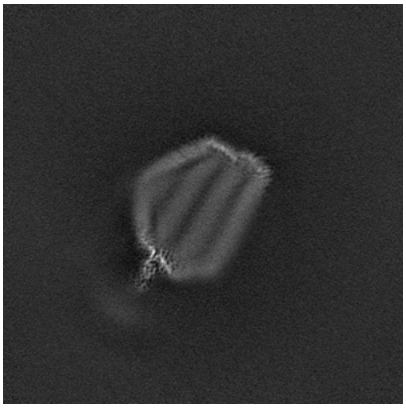
6.3.1 Primary map

X Index: 248

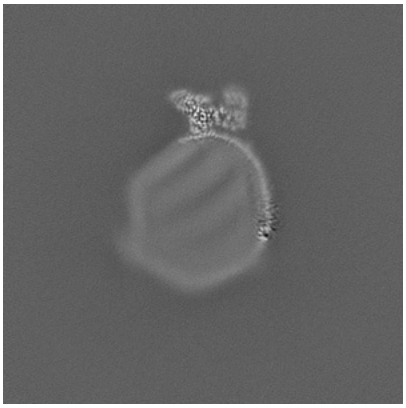
Y Index: 171

Z Index: 160

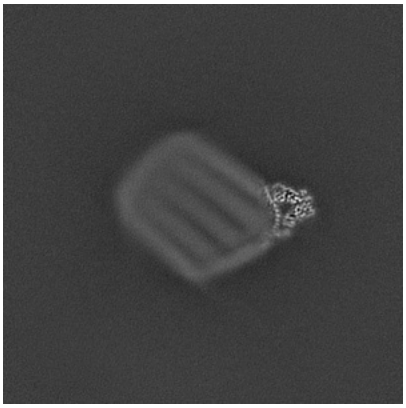
6.3.2 Raw map



X Index: 184



Y Index: 172

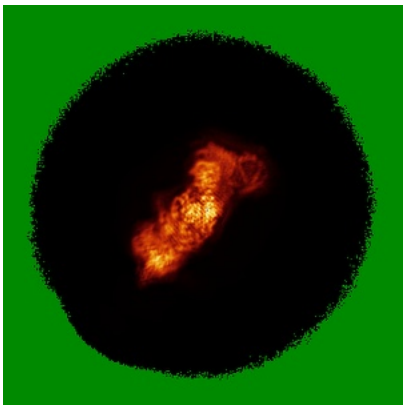


Z Index: 163

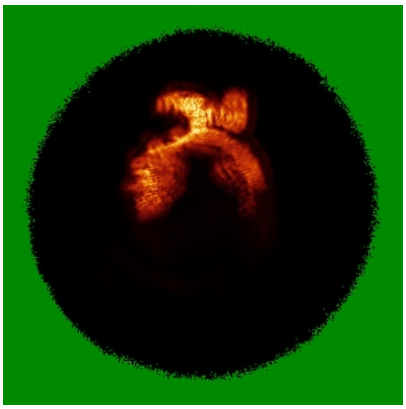
The images above show the largest variance slices of the map in three orthogonal directions.

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

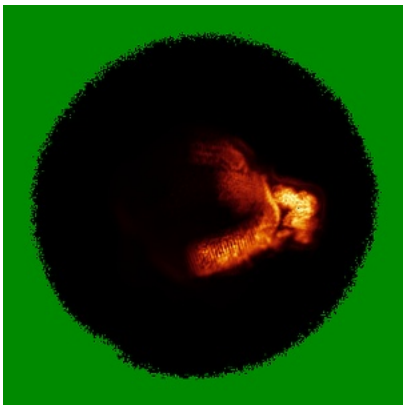
6.4.1 Primary map



X

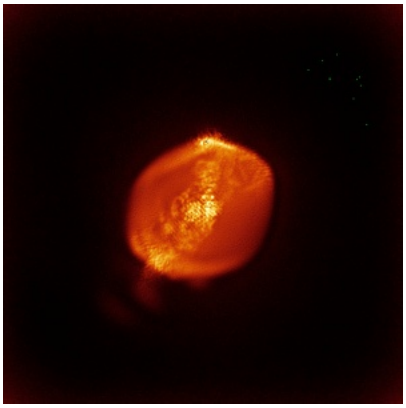


Y

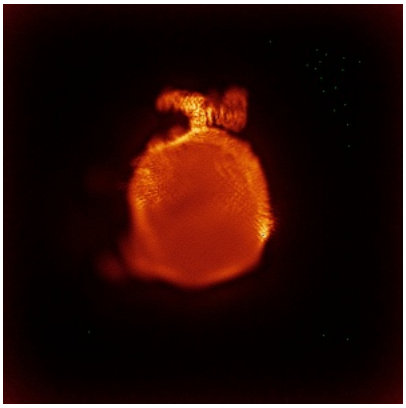


Z

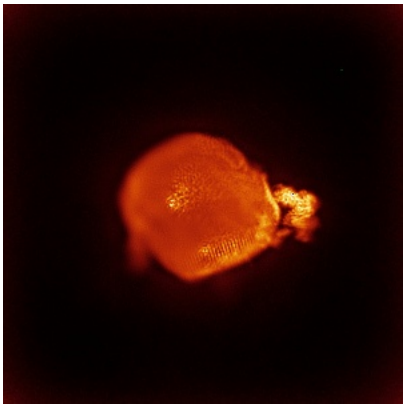
6.4.2 Raw map



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 0.1. 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.

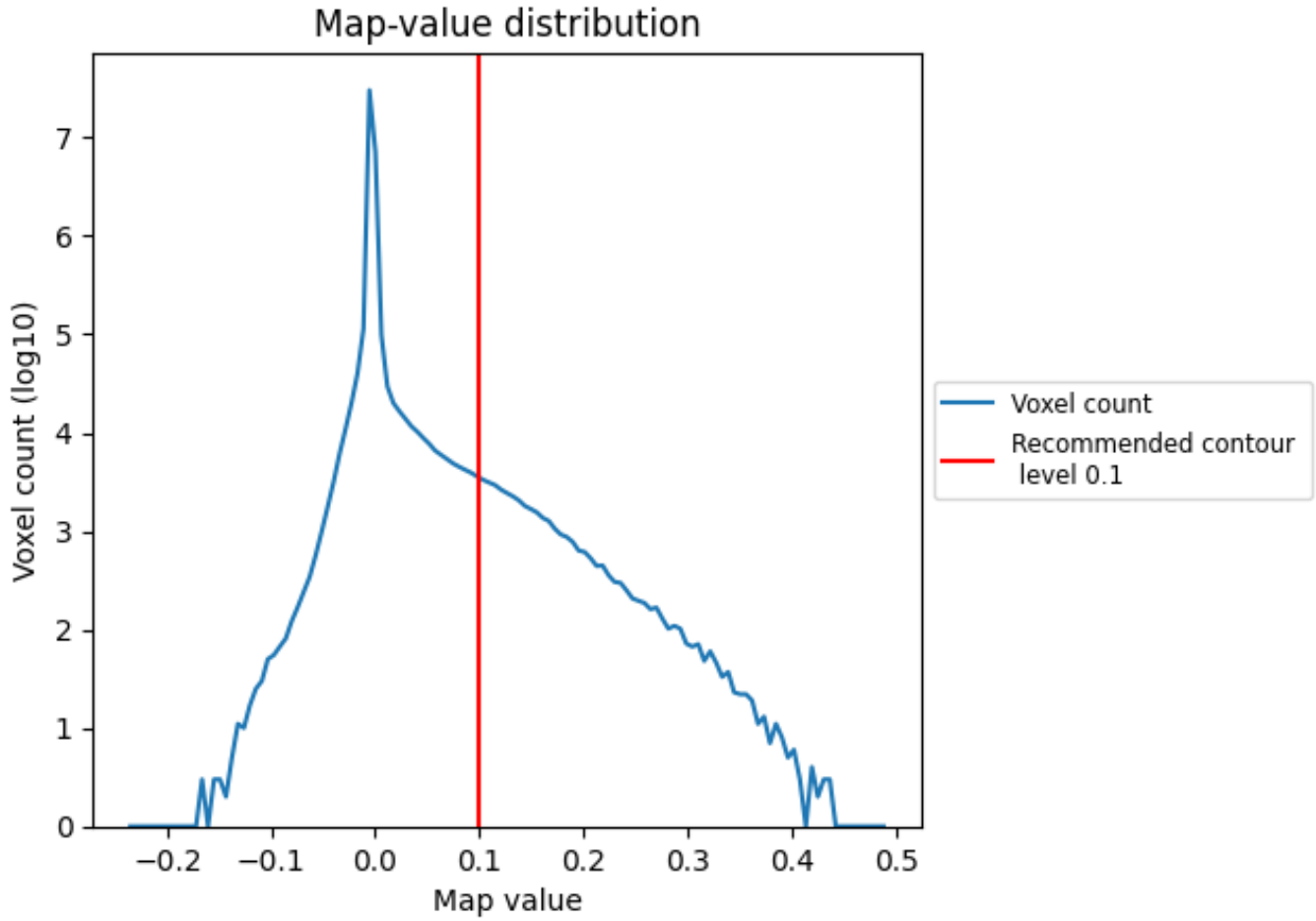
6.6 Mask visualisation (i)

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

7 Map analysis

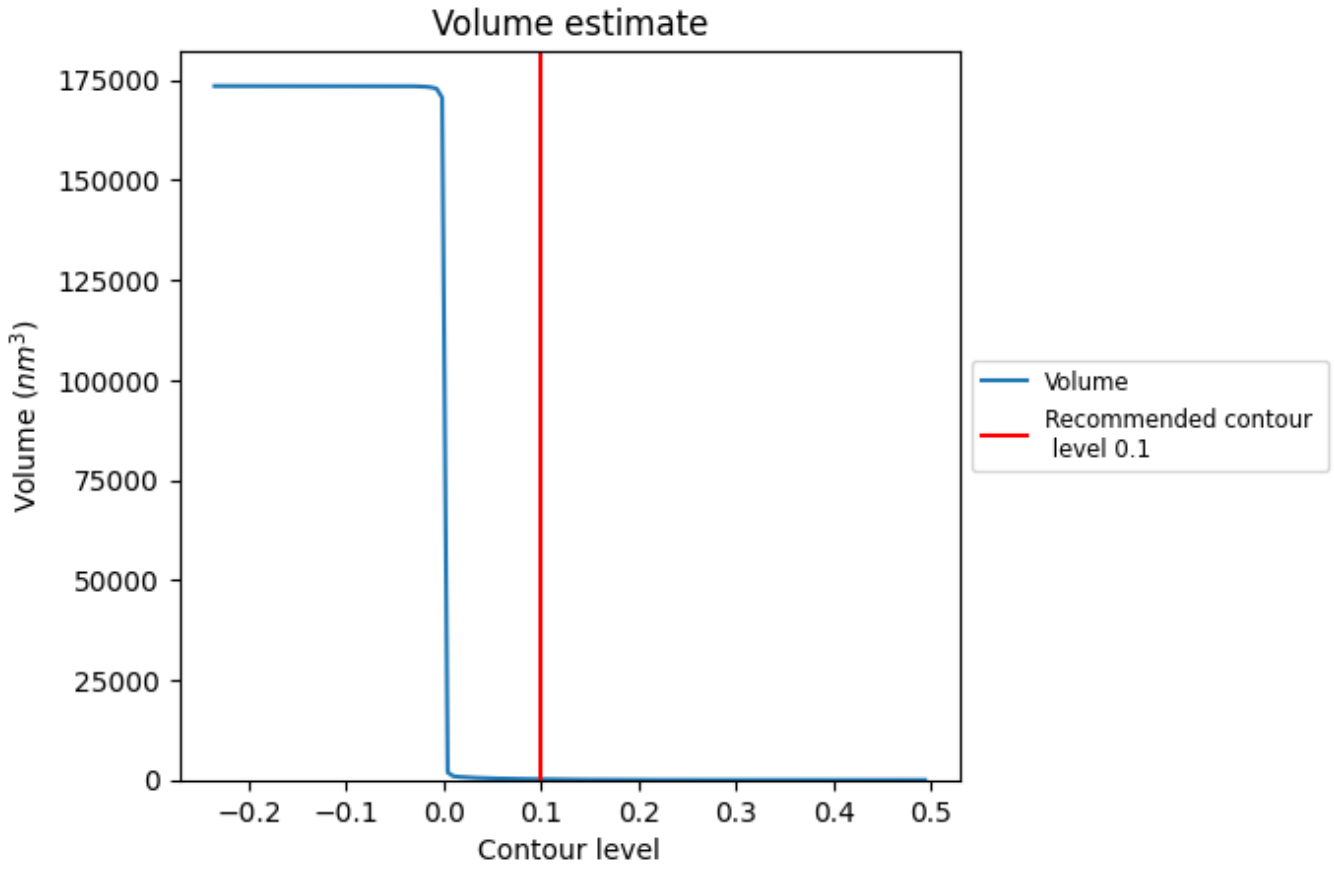
This section contains the results of statistical analysis of the map.

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.

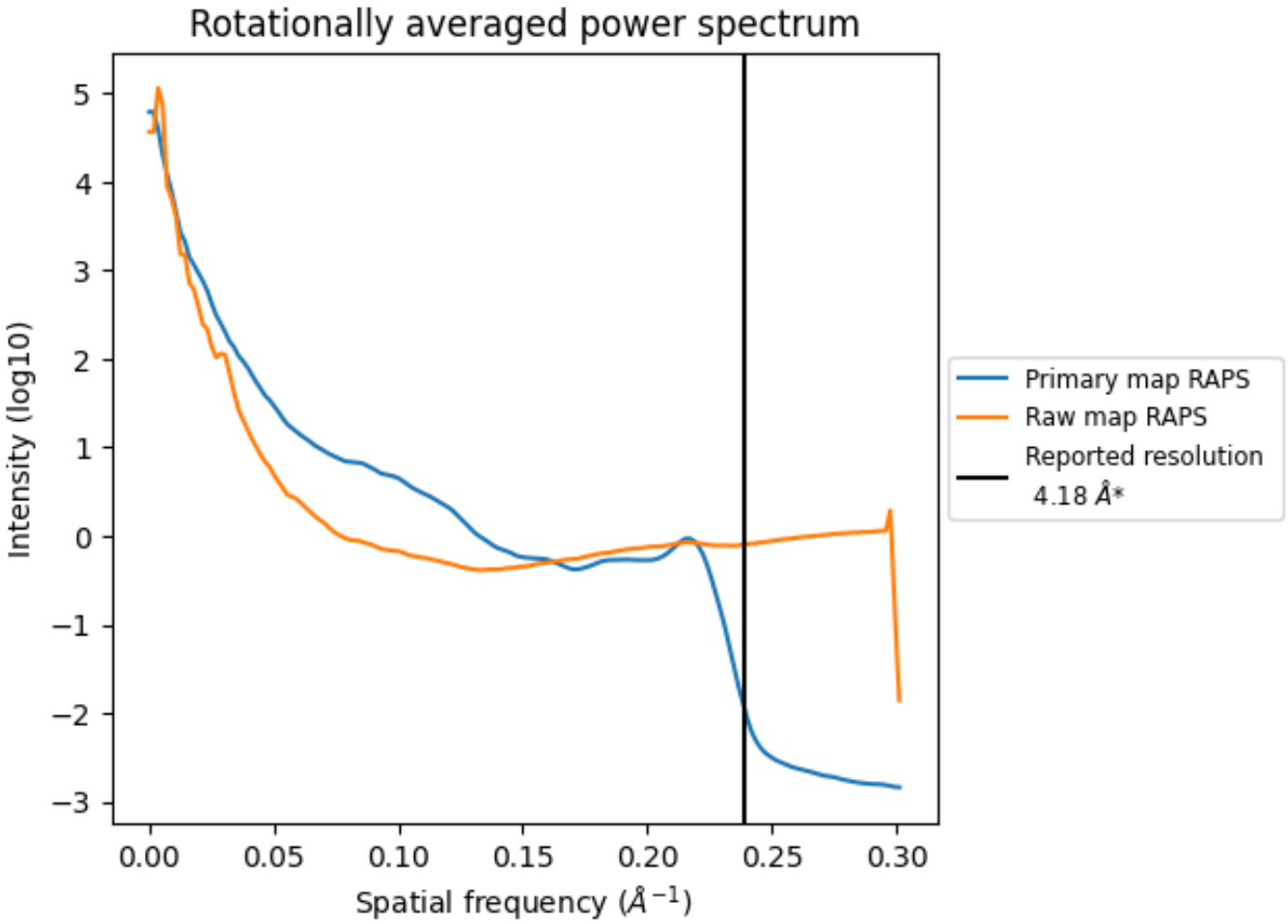
7.2 Volume estimate (i)



The volume at the recommended contour level is 174 nm^3; this corresponds to an approximate mass of 157 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)

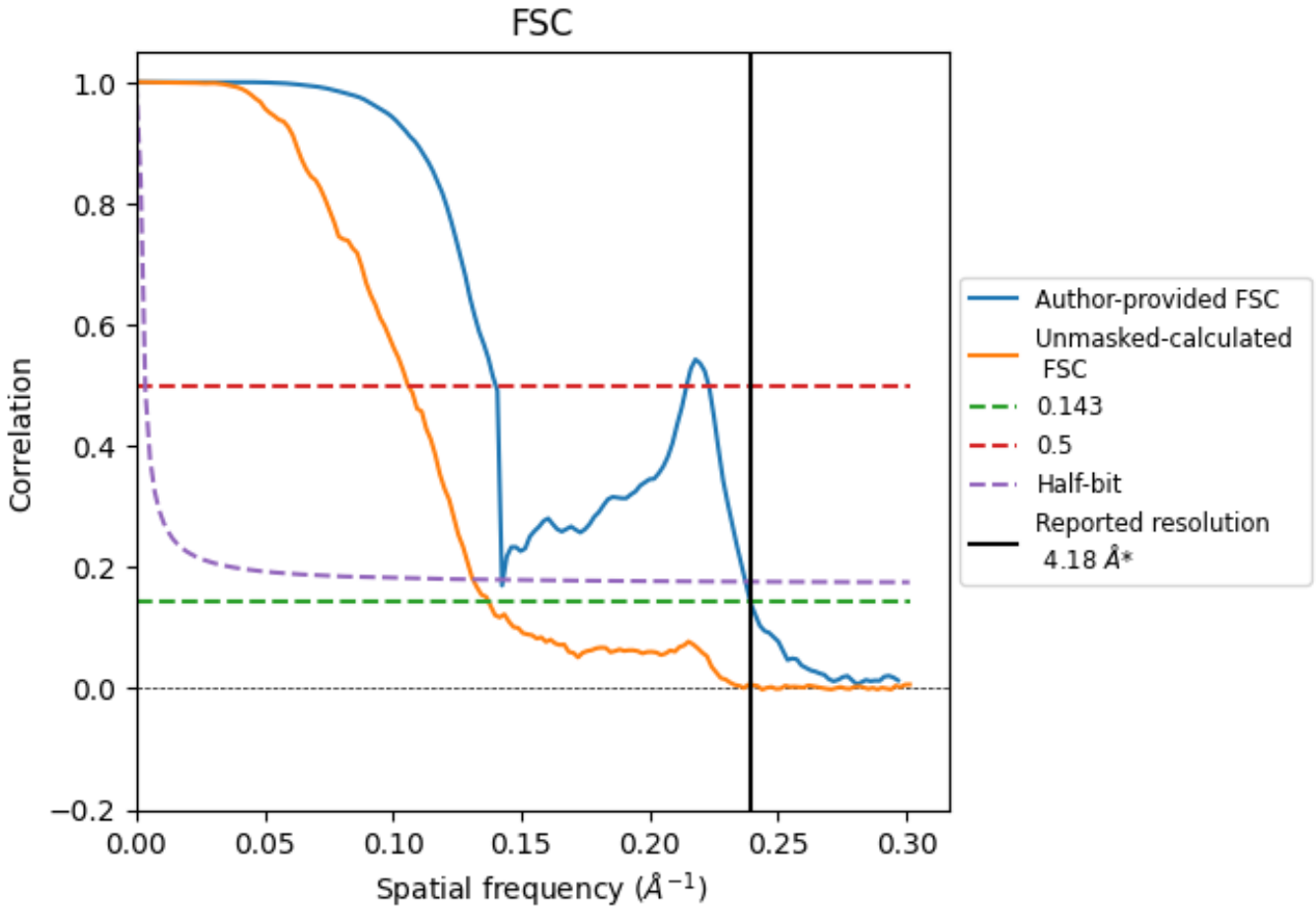


*Reported resolution corresponds to spatial frequency of 0.239 Å^{-1}

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 0.239 Å^{-1}

8.2 Resolution estimates (i)

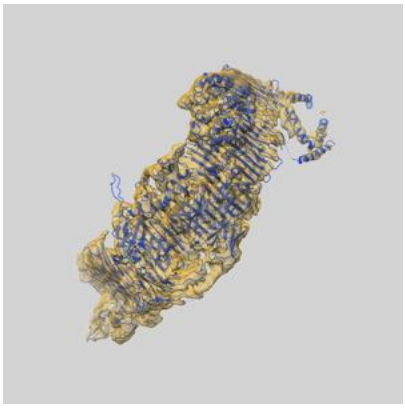
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.18	-	-
Author-provided FSC curve	4.18	7.14	7.02
Unmasked-calculated*	7.29	9.45	7.63

*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 7.29 differs from the reported value 4.18 by more than 10 %

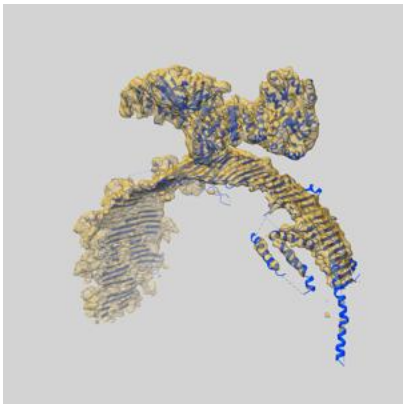
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44450 and PDB model 9BDE. Per-residue inclusion information can be found in section 3 on page 6.

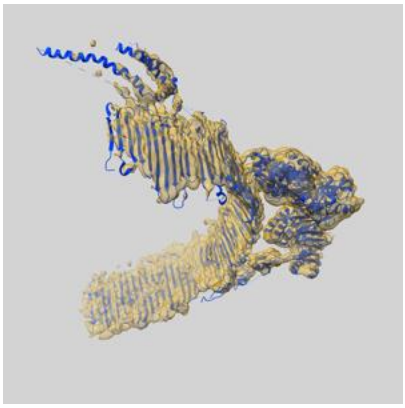
9.1 Map-model overlay



X



Y



Z

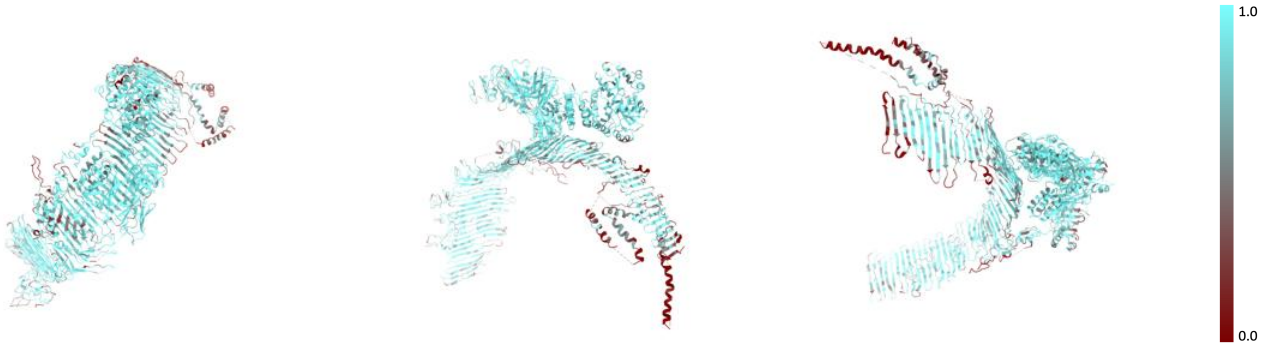
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

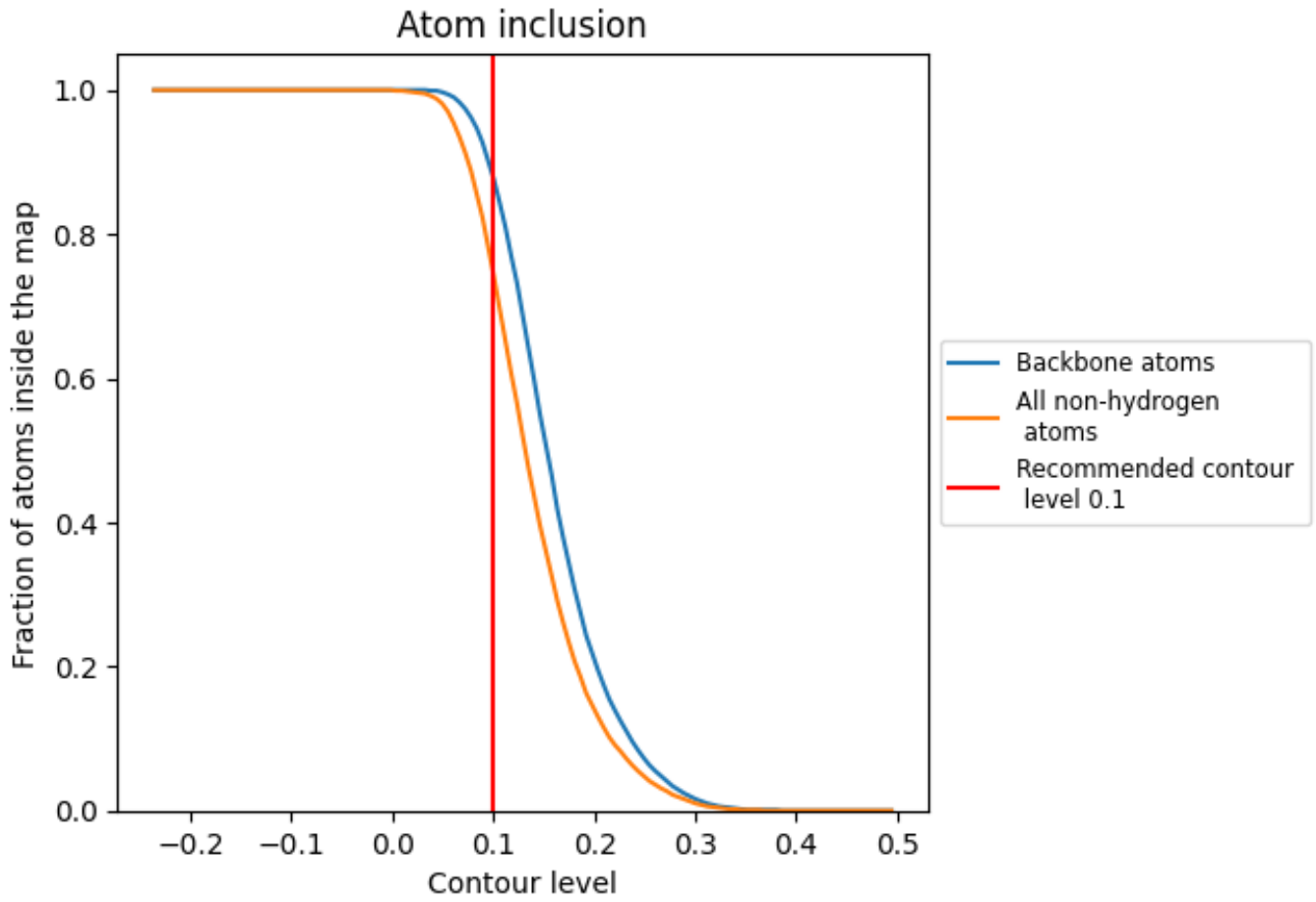
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.3110
A	0.6640	0.3150
B	0.8210	0.2770
H	0.8730	0.3790
L	0.8660	0.3440
N	0.9450	0.4300
R	0.7410	0.2350