wwPDB EM Validation Summary Report

Oct 14, 2024 – 11:41 PM JST

PDB ID	:	8JX9
EMDB ID	:	EMD-36693
Title	:	rat megalin bodyA
Authors	:	Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on	:	2023-06-30
Resolution	:	3.80 Å(reported)
Based on initial model	:	.

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

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

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

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

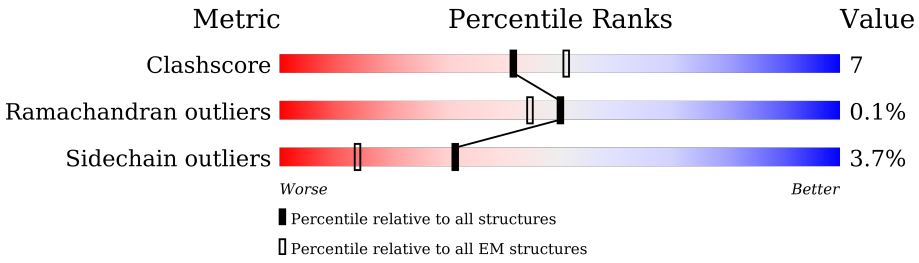
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.80 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	A	4660	7% 7% 92%
1	B	4660	19% 77%
2	O	5	80% 20%
3	C	3	67% 33% 67%
3	D	3	67% 33%
4	E	5	40% 40% 60%
4	H	5	20% 60% 20% 20%
4	I	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
5	F	2	100%
5	G	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11822 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.

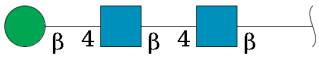
- Molecule 1 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2904	1844	493	549	18		
1	B	1077	Total	C	N	O	S	0	0
			8455	5100	1537	1687	131		

- Molecule 2 is a protein called ligand.

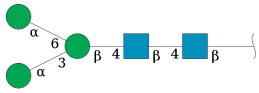
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

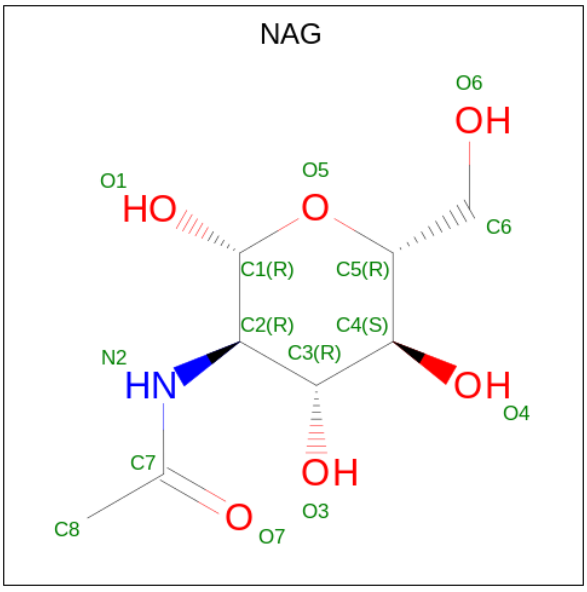


Mol	Chain	Residues	Atoms	AltConf	Trace
4	E	5	Total C N O 61 34 2 25	0	0
4	H	5	Total C N O 61 34 2 25	0	0
4	I	5	Total C N O 61 34 2 25	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	2	Total C N O 28 16 2 10	0	0
5	G	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C N O 14 8 1 5	0

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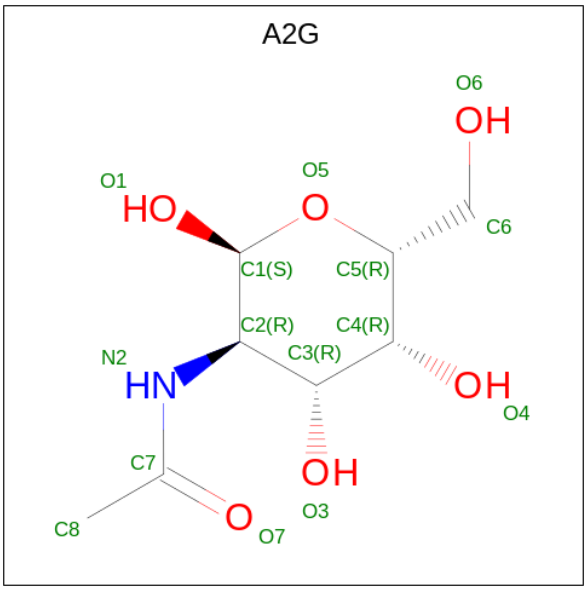
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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

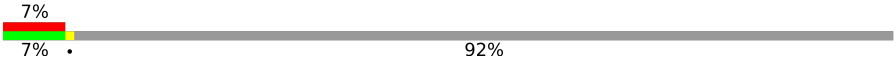
Mol	Chain	Residues	Atoms		AltConf
8	B	20	Total	Ca	0
			20	20	

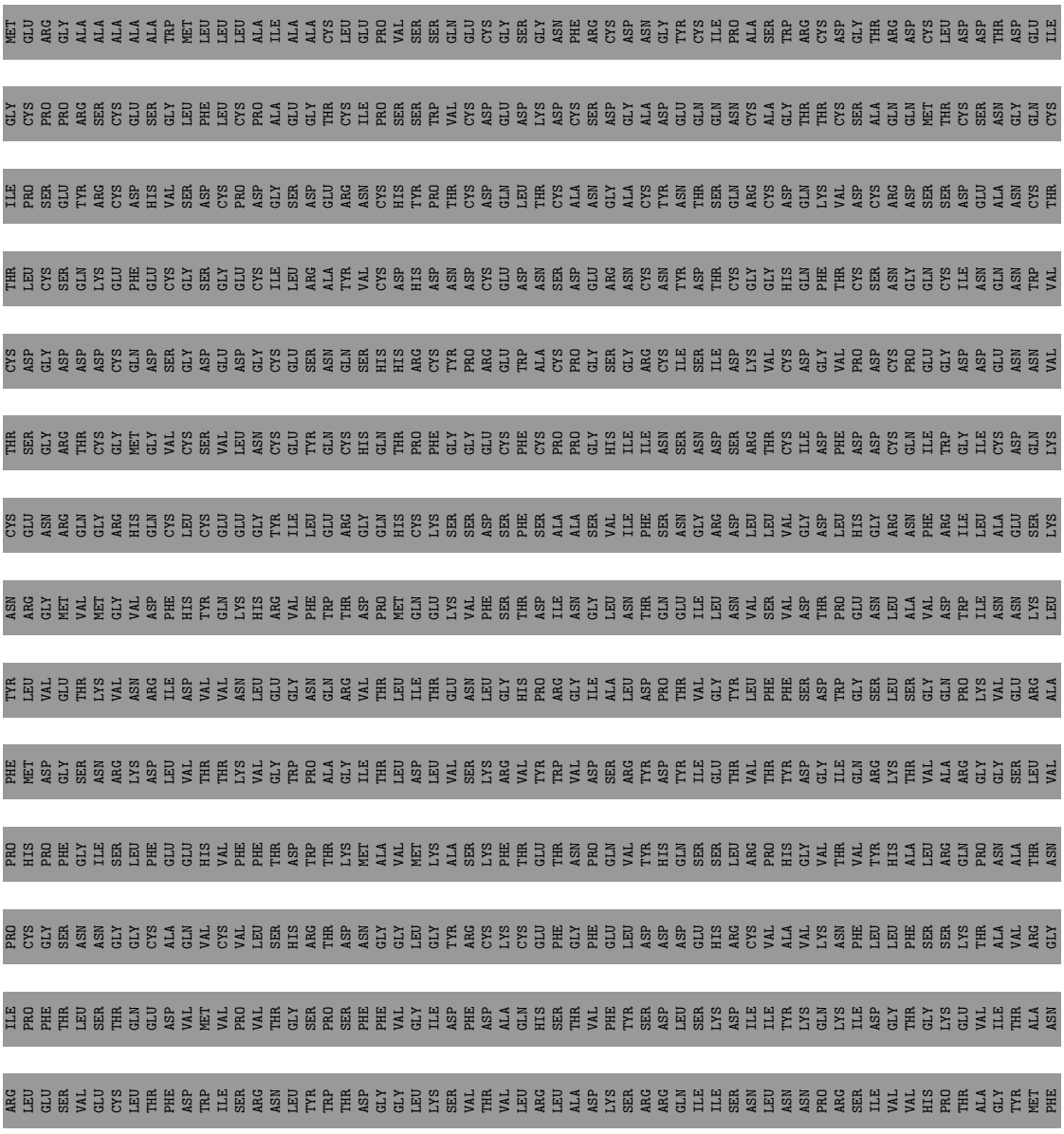
3 Residue-property plots (i)

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: LDL receptor related protein 2

Chain A:





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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

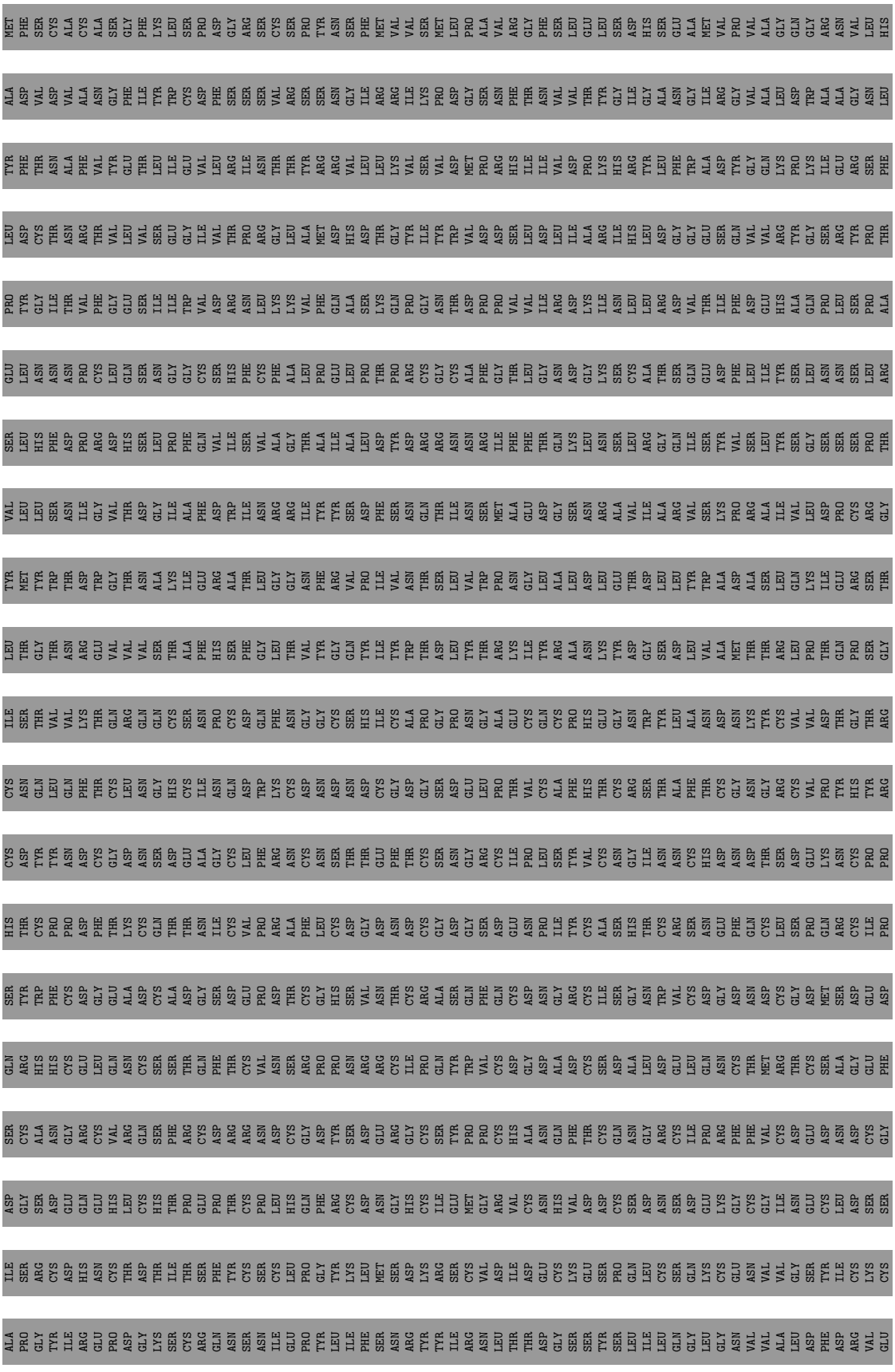
CYS VAL ARG GLY ASP GLN PRO PHE LEU MET SER VAL ARG ASP ASN ILE ILE PHE GLY ILE SER LEU ASP PRO GLU VAL LYS SER ASN ASP ALA MET VAL PRO ILE SER GLY ILE GLN HIS GLY TYR ASP VAL GLU PHE ASP ASP SER GLU GLN PHE ILE TYR TRP VAL GLU ASN PRO GLY

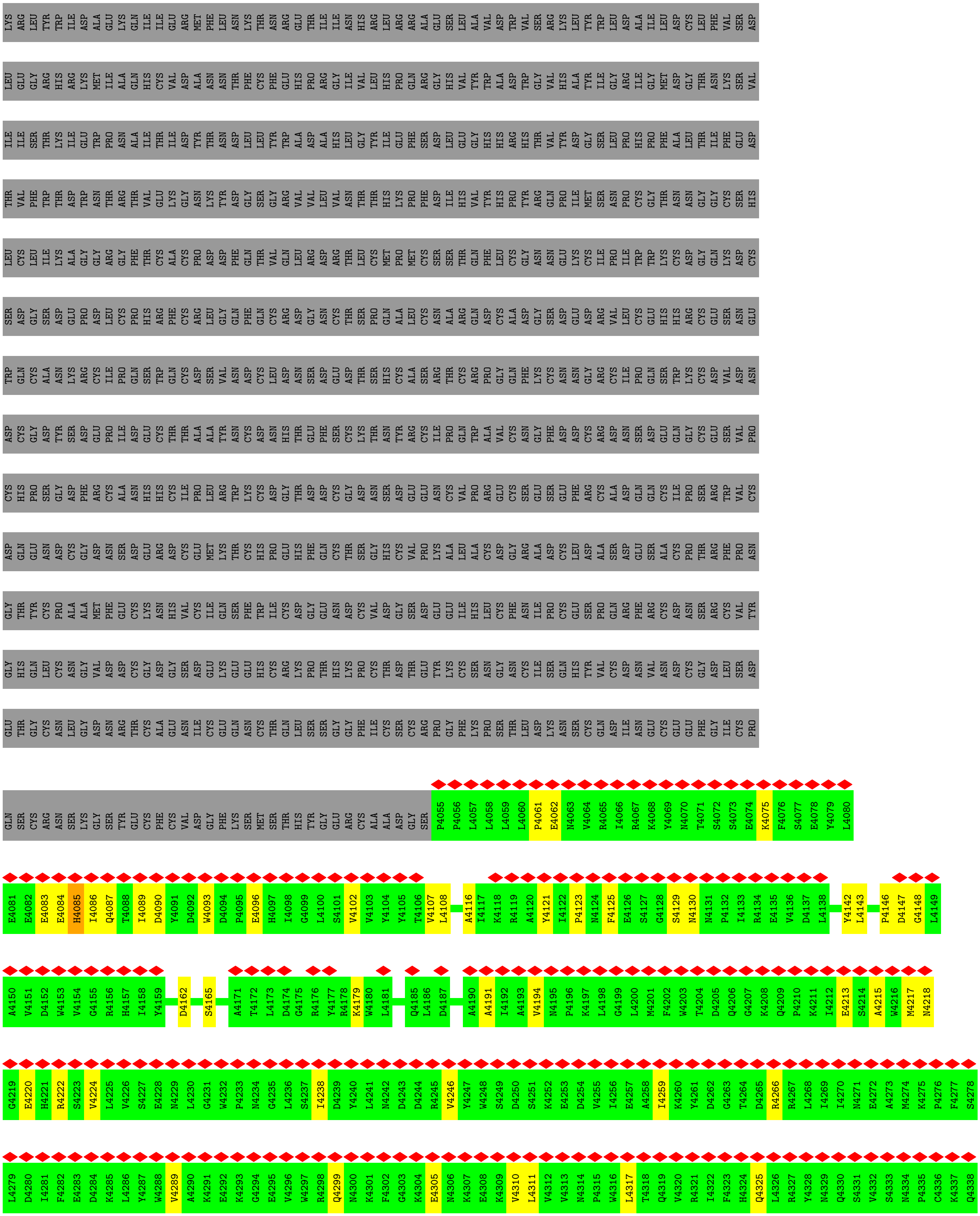
GLU ILE HIS ARG VAL LYS THR ASP GLY SER ASN ARG THR VAL PHE ALA PRO LEU SER LEU LEU GLY SER SER LEU GLY LEU ALA LEU ASP TRP VAL SER ARG ASN ILE TYR TYR THR THR PRO ALA SER ARG SER ILE GLU VAL LEU THR LEU LYS GLY ASP THR ARG TYR GLY LYS THR

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

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

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

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LEU GLU GLY ARG HIS ARG LYS MET ILE ALA GLN HIS CYS VAL ASP ALA ASN ASN THR PHE CYS PHE GLU HIS PRO ARG GLY ILE VAL LEU HIS PRO GLN ARG GLY HIS VAL TYR TRP ALA ASP TRP GLY VAL HIS ALA TYR ILE GLY ARG ILE GLY MET ASP GLY THR ASN LYS SER VAL
ILE ILE SER THR LYS ILE GLU TRP PRO ASN ALA ILE THR ILE ASP TYR THR ASN ASP LEU LEU TYR TRP ALA ASP ALA HIS LEU GLY TYR ILE GLU PHE SER ASP LEU GLU GLY HIS HIS ARG HIS THR VAL TYR ASP GLY SER LEU PRO HIS PRO PHE ALA LEU THR ILE PHE GLU ASP
THR VAL PHE TRP THR ASP TRP ASN THR ARG THR VAL GLU LYS GLY ASN LYS TYR ASP GLY SER GLY ARG VAL VAL LEU VAL ASN THR THR HIS LYS PRO PHE ASP ILE HIS VAL TYR HIS PRO TYR ARG GLN PRO ILE MET SER ASN PRO CYS GLY THR ASN ASN GLY GLY CYS SER HIS
LEU CYS LEU ILE LYS ALA GLY GLY ARG GLY PHE THR CYS ALA CYS PRO ASP ASP PHE GLN THR VAL GLN LEU ARG ASP ARG THR LEU CYS MET PRO MET CYS SER SER THR GLN PHE LEU CYS GLY ASN ASN GLU LYS CYS ILE PRO ILE TRP TRP LYS CYS ASP GLY GLN LYS ASP CYS
SER ASP GLY SER ASP GLU PRO ASP LEU CYS PRO HIS ARG PHE CYS ARG LEU GLY GLN PHE GLN CYS ARG ASP GLY ASN CYS THR SER PRO GLN ALA LEU CYS ASN ALA ARG GLN ASP CYS ALA ASP GLY SER ASP GLU ASP ARG VAL LEU CYS GLU HIS HIS ARG CYS GLU SER ASN GLU
TRP GLN CYS ALA ASN LYS ARG CYS ILE PRO GLN SER TRP GLN CYS ASP SER VAL ASN ASP CYS LEU ASP ASN SER ASP GLU ASP THR SER HIS CYS ALA SER ARG THR CYS ARG PRO GLY GLN PHE LYS CYS ASN ASN GLY ARG CYS ILE PRO GLN SER TRP LYS CYS ASP VAL ASP ASN
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CYS HIS PRO SER GLY ASP PHE ARG CYS ALA ASN HIS HIS CYS ILE PRO LEU ARG TRP LYS CYS ASP GLY THR ASP ASP CYS GLY ASP ASN SER ASP GLU GLU ASN CYS VAL PRO ARG GLU CYS SER GLU SER GLU PHE ARG CYS ALA ASP GLN GLN CYS ILE PRO SER ARG TRP VAL CYS
ASP GLN GLU ASN ASP CYS GLY ASP ASN SER ASP GLU ARG ASP CYS GLU MET LYS THR CYS HIS PRO GLU HIS PHE GLN CYS THR SER GLY HIS CYS VAL PRO LYS ALA LEU ALA CYS ASP GLY ARG ALA ASP CYS LEU ASP ALA SER ASP GLU SER ALA CYS PRO THR ARG PHE PRO ASN
GLY THR TYR CYS PRO ALA ALA MET PHE GLU CYS LYS ASN HIS VAL CYS ILE GLN SER PHE TRP ILE CYS ASP GLY GLU ASN ASP CYS VAL ASP GLY SER ASP GLU GLU ILE HIS LEU CYS PHE ASN ILE PRO CYS GLU SER PRO GLN ARG PHE ARG CYS ASP ASN SER ARG CYS VAL TYR
GLY HIS GLN LEU CYS ASN GLY VAL ASP ASP CYS GLY ASP GLY SER ASP GLU LYS GLU GLU HIS CYS ARG LYS PRO THR HIS LYS PRO CYS THR ASP THR GLU TYR LYS CYS SER ASN GLY ASN CYS ILE SER GLN HIS TYR VAL CYS ASP ASN VAL ASN ASP CYS GLY ASP LEU SER ASP
GLU THR GLY CYS ASN LEU GLY ASP ASN ARG THR CYS ALA GLU ASN ILE CYS GLU GLN ASN CYS THR GLN LEU SER SER GLY GLY PHE ILE CYS SER CYS ARG PRO GLY PHE LYS PRO SER THR LEU ASP LYS ASN SER CYS GLN ASP ILE ASN GLU CYS GLU GLU PHE GLY ILE CYS PRO
GLN SER CYS ARG ASN SER LYS GLY SER TYR GLU CYS PHE CYS VAL ASP GLY PHE LYS SER MET SER THR HIS TYR GLY GLU ARG CYS ALA ALA ASP GLY SER P4055 P4056 L4057 L4058 L4059 L4060 P4061 E4062 N4063 V4064 R4065 I4066 R4067 K4068 Y4069 N4070 T4071 S4072 S4073 E4074 K4075 F4076 S4077 E4078 Y4079 L4080
E4081 E4082 E4083 E4084 H4085 I4086 Q4087 T4088 I4089 D4090 Y4091 D4092 W4093 D4094 P4095 E4096 H4097 I4098 G4099 L4100 S4101 V4102 V4103 Y4104 Y4105 T4106 V4107 L4108 A4116 I4117 K4118 R4119 A4120 Y4121 I4122 P4123 N4124 F4125 E4126 S4127 G4128 S4129 N4130 N4131 P4132 I4133 R4134 E4135 V4136 D4137 L4138 Y4142 L4143 P4146 D4147 G4148 L4149
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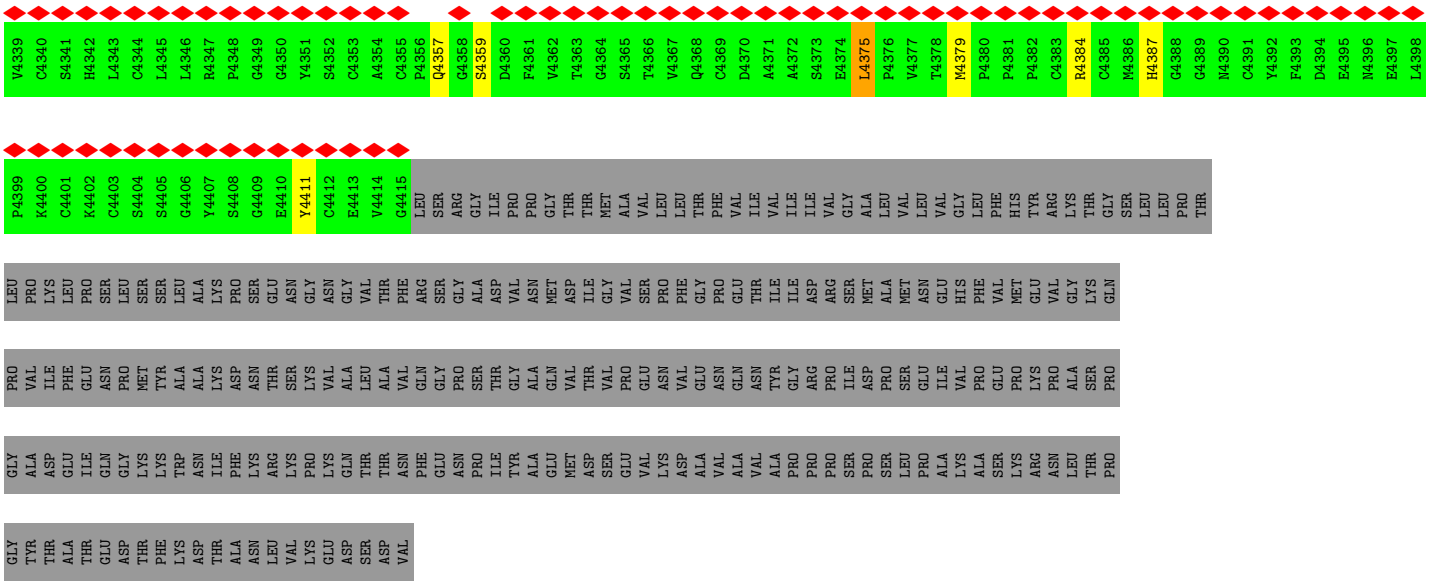
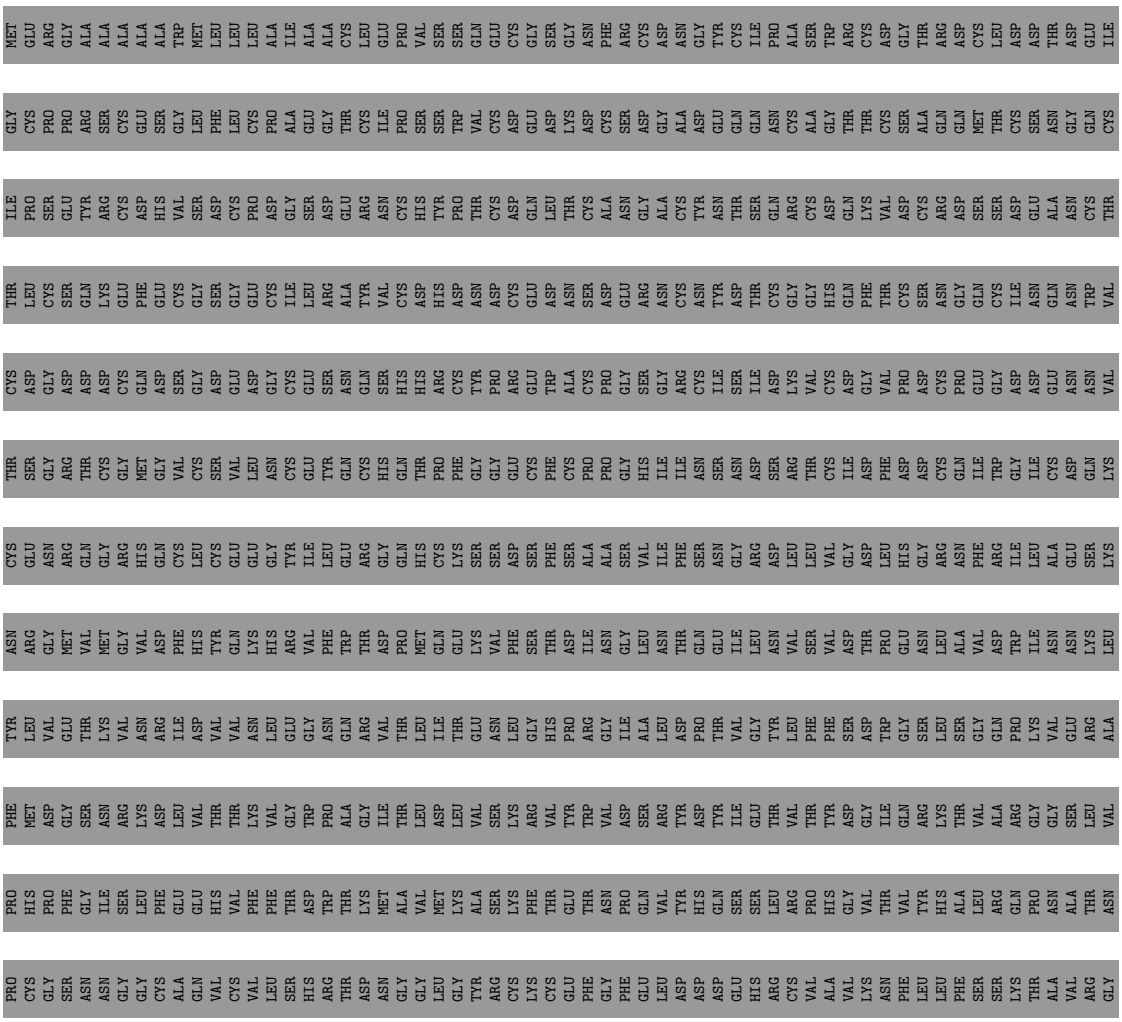
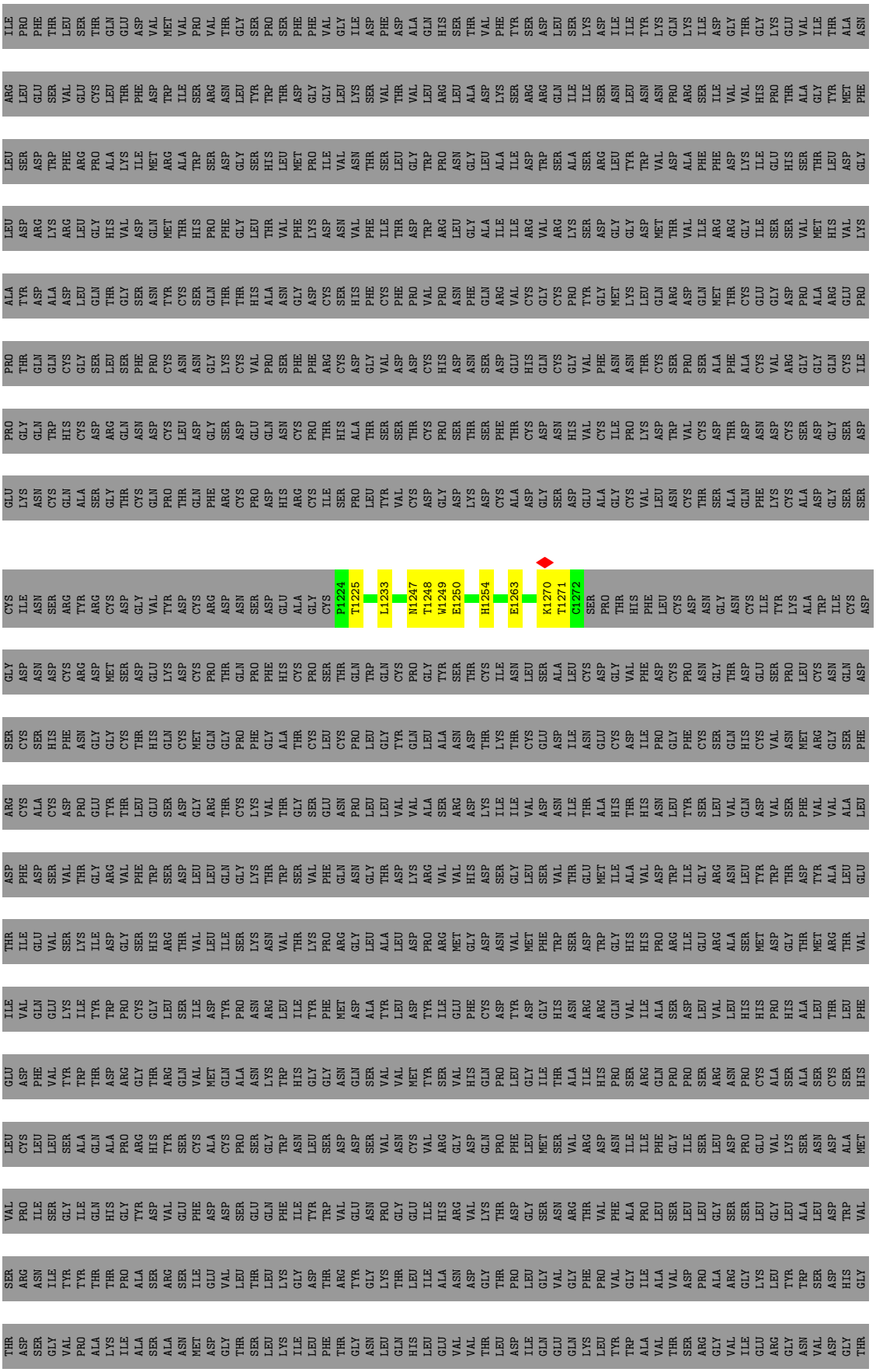
G4219 E4220 H4221 R4222 S4223 V4224 L4225 V4226 S4227 E4228 N4229 L4230 G4231 W4232 P4233 N4234 G4235 L4236 S4237 I4238 D4239 Y4240 L4241 N4242 D4243 D4244 R4245 V4246 Y4247 W4248 S4249 D4250 S4251 K4252 E4253 D4254 V4255 I4256 E4257 A4258 I4259 K4260 Y4261 D4262 G4263 T4264 D4265 R4266 R4267 L4268 I4269 I4270 N4271 E4272 A4273 M4274 K4275 P4276 F4277 S4278
L4279 D4280 I4281 F4282 E4283 D4284 K4285 L4286 Y4287 W4288 V4289 A4290 K4291 E4292 K4293 G4294 E4295 V4296 W4297 R4298 Q4299 N4300 K4301 F4302 G4303 K4304 E4305 N4306 K4307 E4308 K4309 V4310 L4311 V4312 V4313 N4314 P4315 W4316 L4317 T4318 Q4319 V4320 R4321 I4322 F4323 H4324 Q4325 L4326 R4327 Y4328 N4329 Q4330 S4331 V4332 S4333 N4334 P4335 C4336 K4337 Q4338



• Molecule 1: LDL receptor related protein 2

Chain B:

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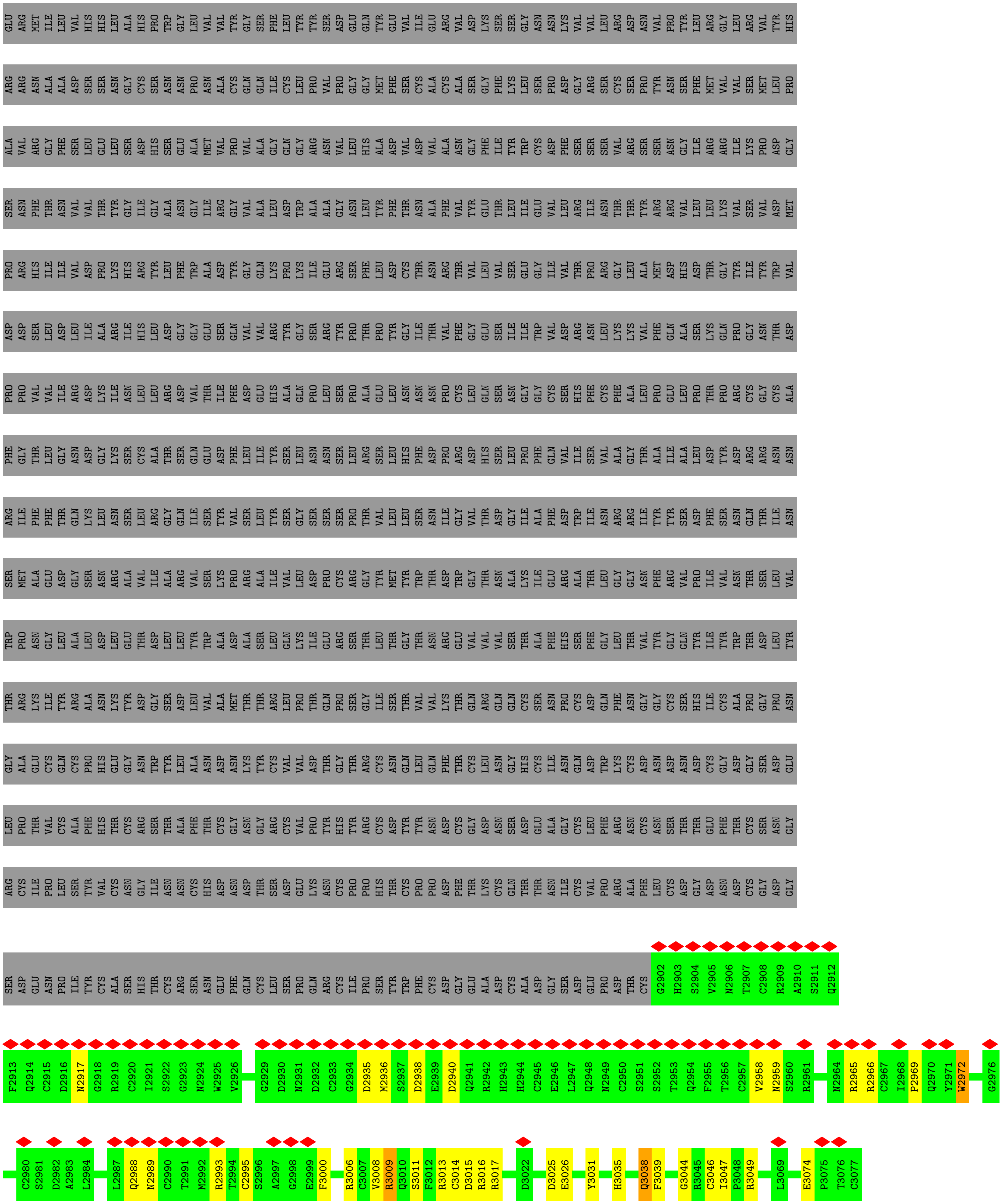
C1272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ARG ARG ASN ALA ALA ASP SER SER ASN GLY CYS SER ASN ASN PRO ASN ALA CYS GLN GLN ILE CYS LEU PRO VAL PRO GLY GLY MET PHE SER CYS ALA CYS ALA SER GLY PHE LYS LEU SER PRO ASP GLY ARG SER CYS SER PRO TYR ASN SER PHE MET VAL VAL SER MET LEU PRO
ALA VAL ARG GLY PHE SER LEU GLU LEU SER ASP HIS SER GLU ALA MET VAL PRO VAL ALA GLY GLN GLY ARG ASN VAL LEU HIS ALA ASP VAL ASP VAL ALA ASN GLY PHE ILE TYR TRP CYS ASP PHE SER SER SER VAL ARG SER SER ASN GLY ILE ARG ARG ILE LYS PRO ASP GLY
SER ASN PHE THR ASN VAL VAL THR TYR GLY ILE GLY ALA ASN GLY ILE ARG GLY VAL ALA LEU ASP TRP ALA ALA GLY ASN LEU TYR PHE THR ASN ALA PHE VAL TYR GLU THR LEU ILE GLU VAL LEU ARG ILE ASN THR THR TYR ARG ARG VAL LEU LEU LYS VAL SER VAL ASP MET
PRO ARG HIS ILE ILE VAL ASP PRO LYS HIS ARG TYR LEU PHE TRP ALA ASP TYR GLY GLN LYS PRO LYS ILE GLU ARG SER PHE LEU ASP CYS THR ASN ARG THR VAL LEU VAL SER GLU GLY ILE VAL THR PRO ARG GLY LEU ALA MET ASP HIS ASP THR GLY TYR ILE TYR TRP VAL
ASP ASP SER LEU ASP LEU ILE ALA ARG ILE HIS LEU ASP GLY GLY GLU SER GLN VAL VAL ARG TYR GLY SER ARG TYR PRO THR PRO TYR GLY ILE THR VAL PHE GLY GLU SER ILE ILE TRP VAL ASP ARG ASN LEU LYS LYS VAL PHE GLN ALA SER LYS GLN PRO GLY ASN THR ASP
PRO PRO VAL VAL ILE ARG ASP LYS ILE ASN LEU LEU ARG ASP VAL THR ILE PHE ASP GLU HIS ALA GLN PRO LEU SER PRO ALA GLU LEU ASN ASN ASN PRO CYS LEU GLN SER ASN GLY GLY CYS SER HIS PHE CYS PHE ALA LEU PRO GLU LEU PRO THR PRO ARG CYS GLY CYS ALA
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ARG ILE PHE PHE THR GLN LYS LEU ASN SER LEU ARG GLY GLN ILE SER TYR VAL SER LEU TYR SER GLY SER SER SER PRO THR VAL LEU LEU SER ASN ILE GLY VAL THR ASP GLY ILE ALA PHE ASP TRP ILE ASN ARG ARG ILE TYR TYR SER ASP PHE SER ASN GLN THR ILE ASN
SER MET ALA GLU ASP GLY SER ASN ARG ALA VAL ILE ALA ARG VAL SER LYS PRO ARG ALA ILE VAL LEU ASP PRO CYS ARG GLY TYR MET TYR TRP THR ASP TRP GLY THR ASN ALA LYS ILE GLU ARG ALA THR LEU GLY GLY ASN PHE ARG VAL PRO ILE VAL ASN THR SER LEU VAL
TRP PRO ASN GLY LEU ALA LEU ASP LEU GLU THR ASP LEU LEU TYR TRP ALA ASP ALA SER LEU GLN LYS ILE GLU ARG SER THR LEU THR GLY THR ASN ARG GLU VAL VAL VAL SER THR ALA PHE HIS SER PHE GLY LEU THR VAL TYR GLY GLN TYR ILE TYR TRP THR ASP LEU TYR
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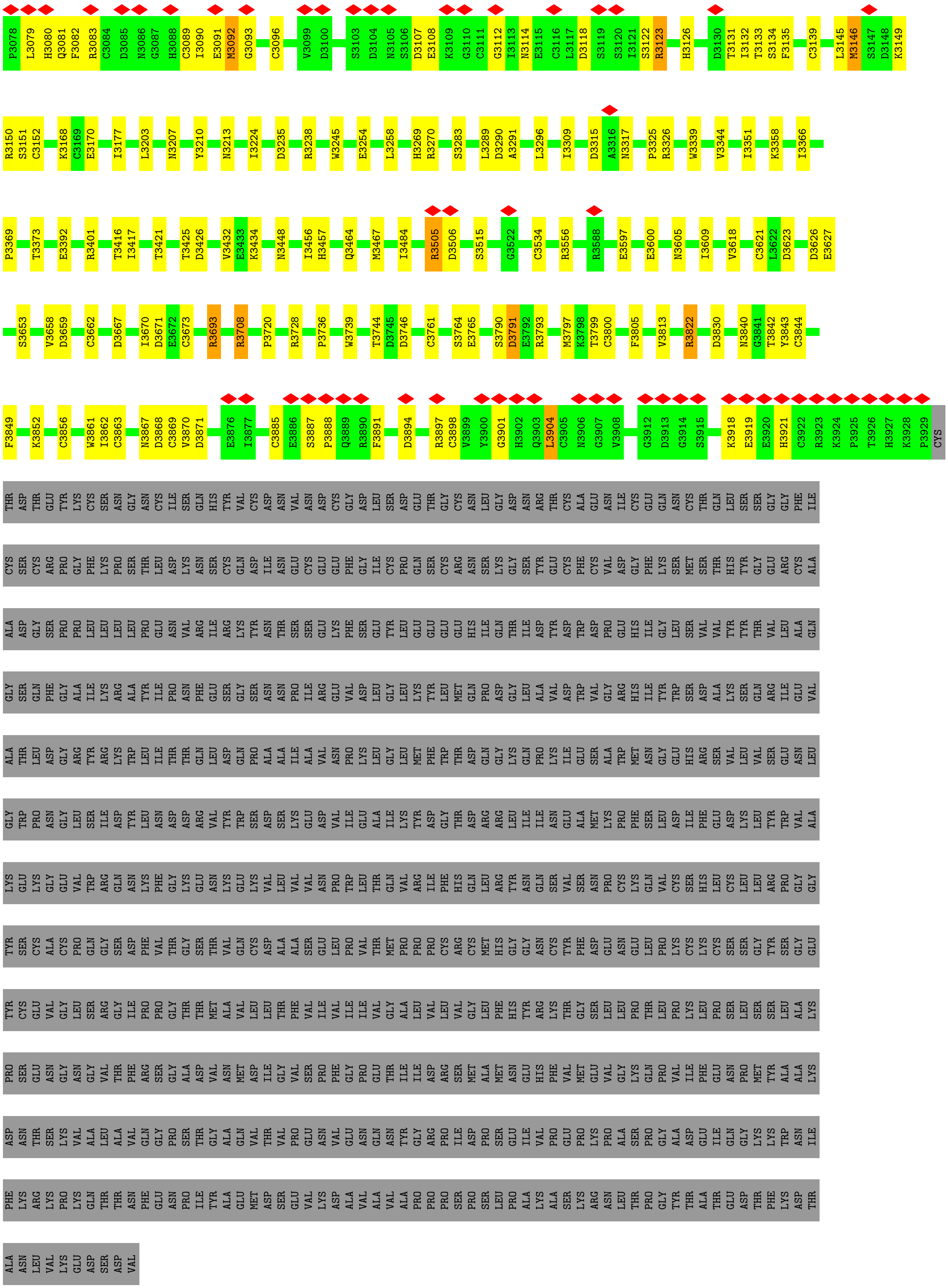
GLY ALA GLU CYS GLN CYS PRO HIS GLU GLY ASN TRP TYR LEU ALA ASN ASP ASN LYS TYR CYS VAL VAL ASP THR GLY THR ARG CYS ASN GLN LEU GLN PHE THR CYS LEU ASN GLY HIS CYS ILE ASN GLN ASP TRP LYS CYS ASP ASN ASP ASN ASP CYS GLY ASP GLY SER ASP GLU
LEU PRO THR VAL CYS ALA PHE HIS THR CYS ARG SER THR ALA PHE THR CYS GLY ASN GLY ARG CYS VAL PRO TYR HIS TYR ARG CYS ASP TYR TYR ASN ASP CYS GLY ASP ASN SER ASP GLU ALA GLY CYS LEU PHE ARG ASN CYS ASN SER THR THR GLU PHE THR CYS SER ASN GLY
ARG CYS ILE PRO LEU SER TYR VAL CYS ASN GLY ILE ASN ASN CYS HIS ASP ASN ASP THR SER ASP GLU LYS ASN CYS PRO PRO HIS THR CYS PRO PRO ASP PHE THR LYS CYS GLN THR THR ASN ILE CYS VAL PRO ARG ALA PHE LEU CYS ASP GLY ASP ASN ASP CYS GLY ASP GLY
SER ASP GLU ASN PRO ILE TYR CYS ALA SER HIS THR CYS ARG SER ASN GLU PHE GLN CYS LEU SER PRO GLN ARG CYS ILE PRO SER TYR TRP PHE CYS ASP GLY GLU ALA ASP CYS ALA ASP GLY SER ASP GLU PRO ASP THR CYS G2902 H2903 S2904 V2905 N2906 T2907 C2908 R2909 A2910 S2911 Q2912
F2913 Q2914 C2915 D2916 N2917 G2918 R2919 C2920 I2921 S2922 G2923 N2924 W2925 V2926 G2929 D2930 N2931 D2932 C2933 G2934 D2935 M2936 S2937 D2938 E2939 D2940 Q2941 R2942 H2943 H2944 C2945 E2946 L2947 Q2948 N2949 C2950 S2951 S2952 T2953 Q2954 F2955 T2956 C2957 V2958 N2959 S2960 R2961 N2964 R2965 R2966 C2967 I2968 P2969 Q2970 Y2971 W2972 G2976
C2980 S2981 D2982 A2983 L2984 L2987 Q2988 N2989 C2990 T2991 M2992 R2993 T2994 C2995 S2996 A2997 G2998 E2999 F3000 R3006 C3007 V3008 R3009 Q3010 S3011 F3012 R3013 C3014 D3015 R3016 R3017 D3022 D3025 E3026 Y3031 H3035 Q3038 F3039 G3044 R3045 C3046 I3047 P3048 R3049 L3069 E3074 P3075 T3076 C3077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R3150 S3151 C3152 K3168 C3169 E3170 I3177 L3203 N3207 Y3210 N3213 I3224 D3235 R3238 W3245 E3254 L3258 H3269 R3270 S3283 L3289 D3290 A3291 L3296 I3309 D3315 A3316 N3317 P3325 R3326 W3339 V3344 I3351 K3358 I3366
P3369 T3373 E3392 R3401 T3416 I3417 T3421 T3425 D3426 V3432 E3433 K3434 N3448 I3456 H3457 Q3464 M3467 I3484 R3505 D3506 S3515 G3522 C3534 R3556 R3588 E3597 E3600 N3605 I3609 V3618 C3621 L3622 D3623 D3626 E3627
S3653 V3658 D3659 C3662 D3667 I3670 D3671 E3672 C3673 R3693 R3708 P3720 R3728 P3736 W3739 T3744 D3745 D3746 C3761 S3764 E3765 S3790 D3791 E3792 R3793 M3797 K3798 T3799 C3800 F3805 V3813 R3822 D3830 N3840 G3841 T3842 Y3843 C3844
F3849 K3852 C3856 W3861 I3862 C3863 N3867 D3868 C3869 V3870 D3871 E3876 I3877 C3885 E3886 S3887 P3888 Q3889 R3890 F3891 D3894 R3897 C3898 V3899 Y3900 G3901 H3902 Q3903 L3904 C3905 N3906 G3907 V3908 G3912 D3913 G3914 S3915 K3918 E3919 E3920 H3921 C3922 R3923 K3924 P3925 T3926 H3927 K3928 P3929 CYS
THR ASP THR GLU TYR LYS CYS SER ASN GLY ASN CYS ILE SER GLN HIS TYR VAL CYS ASP ASN VAL ASN ASP CYS GLY ASP LEU SER ASP GLU THR GLY CYS ASN LEU GLY ASP ASN ARG THR CYS ALA GLU ASN ILE CYS GLU GLN ASN CYS THR GLN LEU SER SER GLY GLY PHE ILE
CYS SER CYS ARG PRO GLY PHE LYS PRO SER THR LEU ASP LYS ASN SER CYS GLN ASP ILE ASN GLU CYS GLU GLU PHE GLY ILE CYS PRO GLN SER CYS ARG ASN SER LYS GLY SER TYR GLU CYS PHE CYS VAL ASP GLY PHE LYS SER MET SER THR HIS TYR GLY GLU ARG CYS ALA
ALA ASP GLY SER PRO PRO LEU LEU LEU LEU PRO GLU ASN VAL ARG ILE ARG LYS TYR ASN THR SER SER GLU LYS PHE SER GLU TYR LEU GLU GLU GLU HIS ILE GLN THR ILE ASP TYR ASP TRP ASP PRO GLU HIS ILE GLY LEU SER VAL VAL TYR TYR THR VAL LEU ALA GLN
GLY SER GLN PHE GLY ALA ILE LYS ARG ALA TYR ILE PRO ASN PHE GLU SER GLY SER ASN ASN PRO ILE ARG GLU VAL ASP LEU GLY LEU LYS TYR LEU MET GLN PRO ASP GLY LEU ALA VAL ASP TRP VAL GLY ARG HIS ILE TYR TRP SER ASP ALA LYS SER GLN ARG ILE GLU VAL
ALA THR LEU ASP GLY ARG TYR ARG LYS TRP LEU ILE THR GLN LEU ASP GLN PRO ALA ALA ILE ALA VAL ASN PRO LYS LEU GLY LEU MET PHE TRP THR ASP GLN GLY LYS GLN PRO LYS ILE GLU SER ALA TRP MET ASN GLY GLU HIS ARG SER VAL LEU VAL SER GLU ASN LEU
GLY TRP PRO ASN GLY LEU SER ILE ASP TYR LEU ASN ASP ASP ARG VAL TYR TRP SER ASP SER LYS GLU ASP VAL ILE GLU ALA ILE LYS TYR ASP GLY THR ASP ARG ARG LEU ILE ILE ASN GLU ALA MET LYS PRO PHE SER LEU ASP ILE PHE GLU ASP LYS LEU TYR TRP VAL ALA
LYS GLU LYS GLY GLU VAL TRP ARG GLN ASN LYS PHE GLY LYS GLU ASN LYS GLU LYS VAL LEU VAL VAL ASN PRO TRP LEU THR GLN VAL ARG ILE PHE HIS GLN LEU ARG TYR ASN GLN SER VAL SER ASN PRO CYS LYS GLN VAL CYS SER HIS LEU CYS LEU LEU ARG PRO GLY GLY
TYR SER CYS ALA CYS PRO GLN GLY SER ASP PHE VAL THR GLY SER THR VAL GLN CYS ASP ALA ALA SER GLU LEU PRO VAL THR MET PRO PRO PRO CYS ARG CYS MET HIS GLY GLY ASN CYS TYR PHE ASP GLU ASN GLU LEU PRO LYS CYS LYS CYS SER SER GLY TYR SER GLY GLU
TYR CYS GLU VAL GLY LEU SER ARG GLY ILE PRO PRO GLY THR THR MET ALA VAL LEU LEU THR PHE VAL ILE VAL ILE ILE VAL GLY ALA LEU VAL LEU VAL GLY LEU PHE HIS TYR ARG LYS THR GLY SER LEU LEU PRO THR LEU PRO LYS LEU PRO SER LEU SER SER LEU ALA LYS
PRO SER GLU ASN GLY ASN GLY VAL THR PHE ARG SER GLY ALA ASP VAL ASN MET ASP ILE GLY VAL SER PRO PHE GLY PRO GLU THR ILE ILE ASP ARG SER MET ALA MET ASN GLU HIS PHE VAL MET GLU VAL GLY LYS GLN PRO VAL ILE PHE GLU ASN PRO MET TYR ALA ALA LYS
ASP ASN THR SER LYS VAL ALA LEU ALA VAL GLN GLY PRO SER THR GLY ALA GLN VAL THR VAL PRO GLU ASN VAL GLU ASN GLN ASN TYR GLY ARG PRO ILE ASP PRO SER GLU ILE VAL PRO GLU PRO LYS PRO ALA SER PRO GLY ALA ASP GLU ILE GLN GLY LYS LYS TRP ASN ILE
PHE LYS ARG LYS PRO LYS GLN THR THR ASN PHE GLU ASN PRO ILE TYR ALA GLU MET ASP SER GLU VAL LYS ASP ALA ALA VAL ALA PRO PRO PRO SER PRO SER LEU PRO ALA LYS ALA SER LYS ARG ASN LEU THR PRO GLY TYR THR ALA THR GLU ASP THR PHE LYS ASP THR
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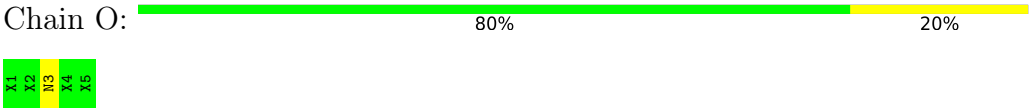
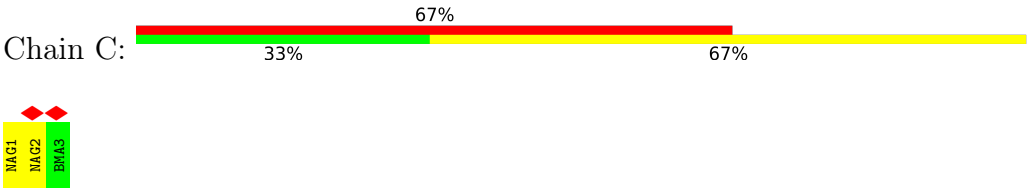
• Molecule 2: ligand

Chain O:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

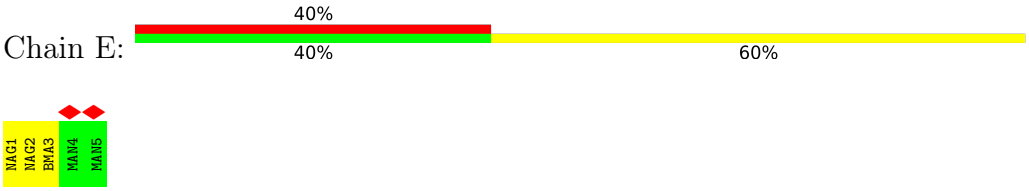


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

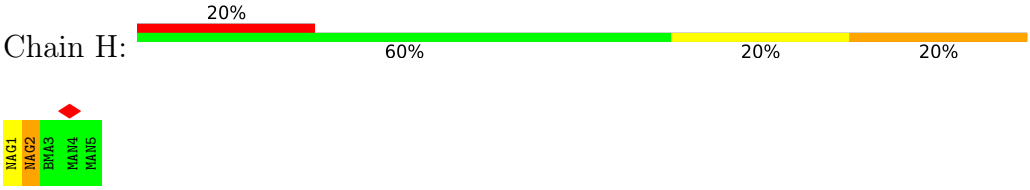
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



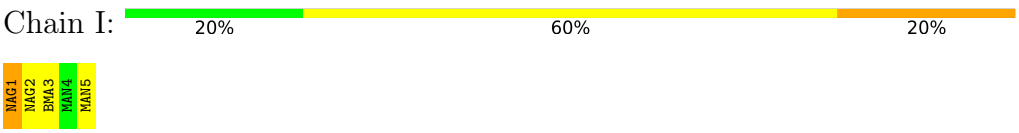
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



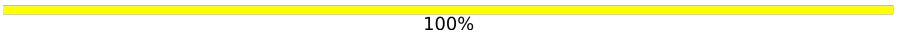
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



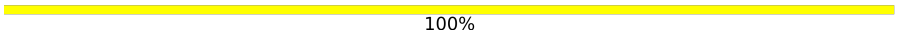
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.411, 1.411, 1.411	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, MAN, A2G, BMA

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	0.24	0/2981	0.49	0/4047
1	B	0.26	0/8659	0.53	0/11737
2	O	0.20	0/7	0.51	0/8
All	All	0.25	0/11647	0.52	0/15792

There are no bond length outliers.

There are no bond angle outliers.

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	2904	0	2797	27	0
1	B	8455	0	7529	120	0
2	O	28	0	12	1	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
4	E	61	0	52	1	0
4	H	61	0	52	1	0
4	I	61	0	52	1	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	1	0
7	B	70	0	60	11	0
8	B	20	0	0	0	0
All	All	11822	0	10698	149	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 7.

The worst 5 of 149 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:1225:THR:OG1	7:B:4703:A2G:C1	1.90	1.19
1:B:3799:THR:OG1	7:B:4706:A2G:C1	1.92	1.18
1:B:1225:THR:CB	7:B:4703:A2G:C1	2.26	1.12
1:B:1225:THR:HB	7:B:4703:A2G:C1	1.83	1.08
1:B:3799:THR:CB	7:B:4706:A2G:C1	2.36	1.03

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	359/4660 (8%)	334 (93%)	25 (7%)	0	100	100
1	B	1073/4660 (23%)	985 (92%)	87 (8%)	1 (0%)	48	79
2	O	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1433/9325 (15%)	1320 (92%)	112 (8%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3123	ARG

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	320/4089 (8%)	309 (97%)	11 (3%)	32 55
1	B	965/4089 (24%)	928 (96%)	37 (4%)	28 52
2	O	1/1 (100%)	1 (100%)	0	100 100
All	All	1286/8179 (16%)	1238 (96%)	48 (4%)	31 53

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3235	ASP
1	B	3505	ARG
1	B	3290	ASP
1	B	3373	THR
1	B	3534	CYS

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

Mol	Chain	Res	Type
1	B	3057	ASN
1	B	3066	GLN
1	B	3602	GLN
1	B	3733	HIS

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)

25 monosaccharides 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	NAG	C	1	1,3	14,14,15	0.44	0	17,19,21	2.39	3 (17%)
3	NAG	C	2	3	14,14,15	0.52	0	17,19,21	1.15	1 (5%)
3	BMA	C	3	3	11,11,12	0.24	0	15,15,17	0.82	0
3	NAG	D	1	1,3	14,14,15	0.37	0	17,19,21	0.87	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	1.13	1 (5%)
3	BMA	D	3	3	11,11,12	0.25	0	15,15,17	0.83	0
4	NAG	E	1	4,1	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.79	0
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	1.15	2 (13%)
4	MAN	E	4	4	11,11,12	0.22	0	15,15,17	0.62	0
4	MAN	E	5	4	11,11,12	0.25	0	15,15,17	0.64	0
5	NAG	F	1	1,5	14,14,15	0.36	0	17,19,21	1.12	1 (5%)
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	1.16	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	1.42	1 (5%)
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.34	0	17,19,21	0.65	0
4	NAG	H	2	4	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
4	BMA	H	3	4	11,11,12	0.29	0	15,15,17	0.82	0
4	MAN	H	4	4	11,11,12	0.25	0	15,15,17	0.70	0
4	MAN	H	5	4	11,11,12	0.23	0	15,15,17	0.67	0
4	NAG	I	1	4,1	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.59	0
4	BMA	I	3	4	11,11,12	0.26	0	15,15,17	1.08	2 (13%)
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.65	0
4	MAN	I	5	4	11,11,12	0.41	0	15,15,17	1.18	2 (13%)

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	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-O5-C5	8.04	123.08	112.19
5	G	1	NAG	C1-O5-C5	5.08	119.08	112.19
3	C	1	NAG	O4-C4-C5	-4.15	98.99	109.30
4	I	1	NAG	C1-O5-C5	3.53	116.98	112.19
3	C	2	NAG	C1-O5-C5	3.07	116.35	112.19

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

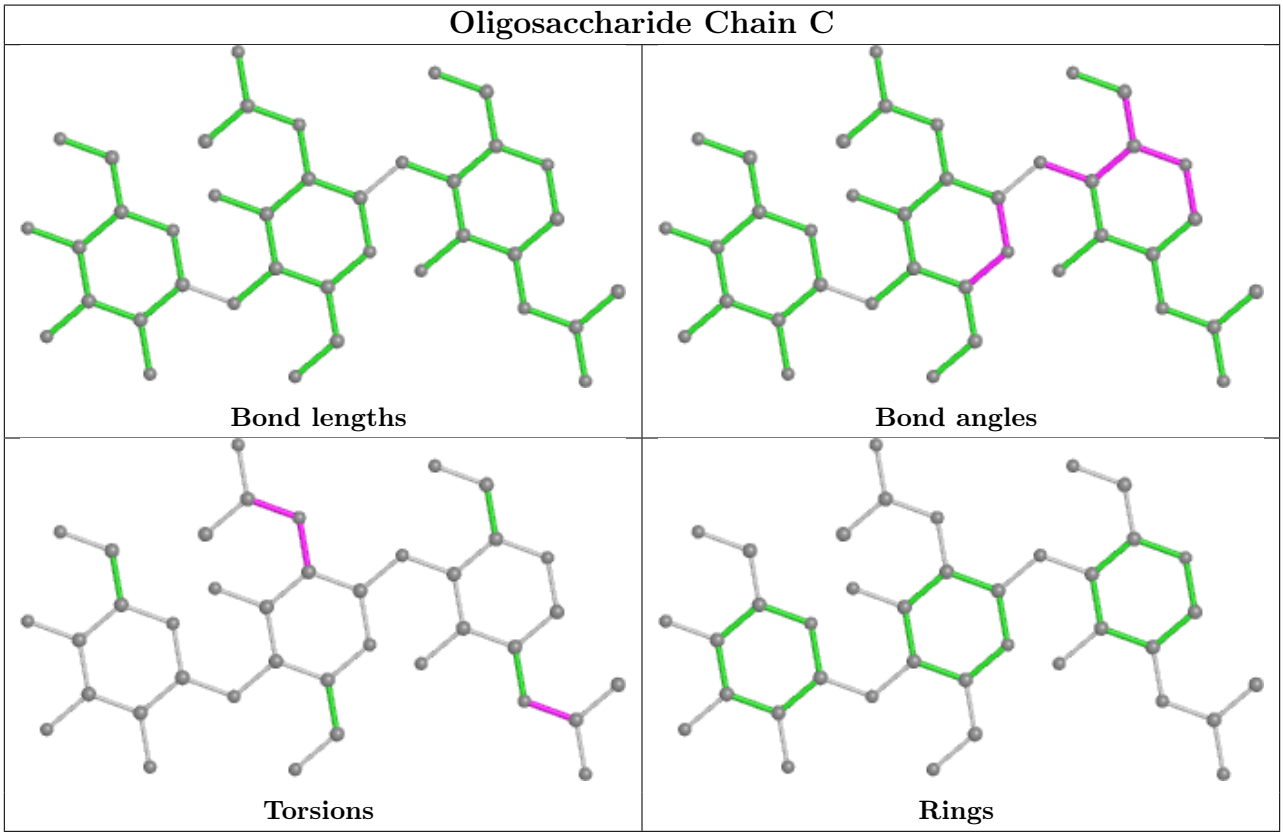
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C8-C7-N2-C2

There are no ring outliers.

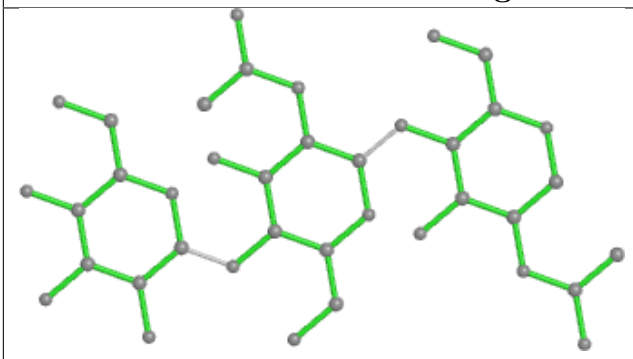
6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	E	1	NAG	1	0
4	H	1	NAG	1	0
4	E	2	NAG	1	0
4	H	2	NAG	1	0
4	I	2	NAG	1	0

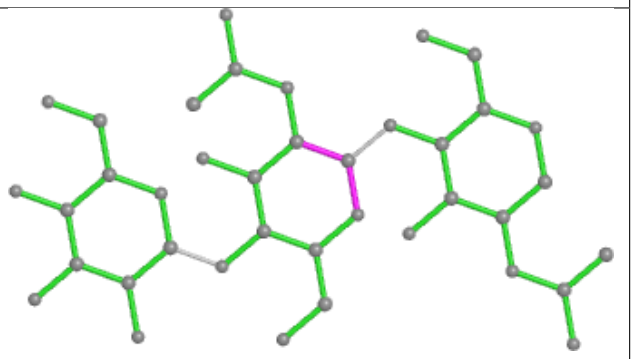
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



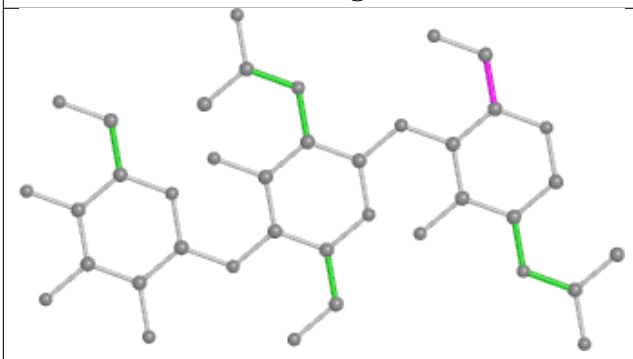
Oligosaccharide Chain D



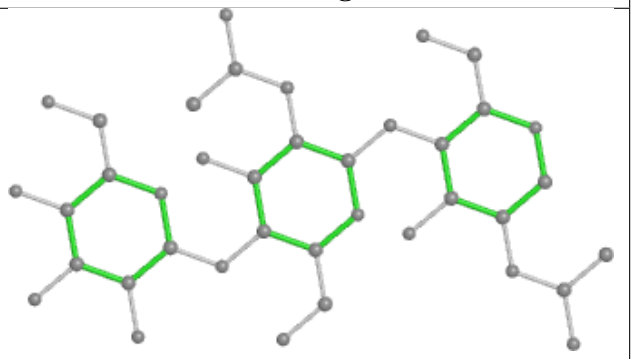
Bond lengths



Bond angles

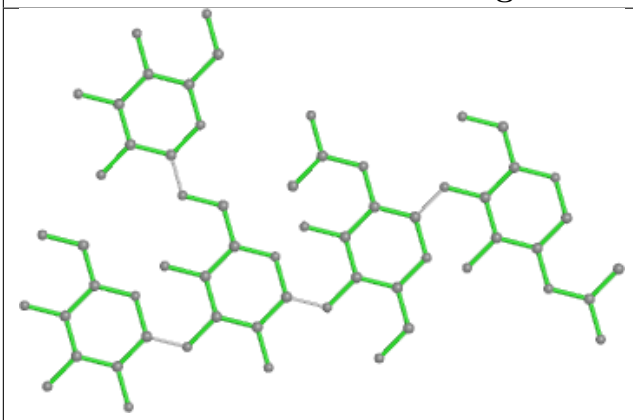


Torsions

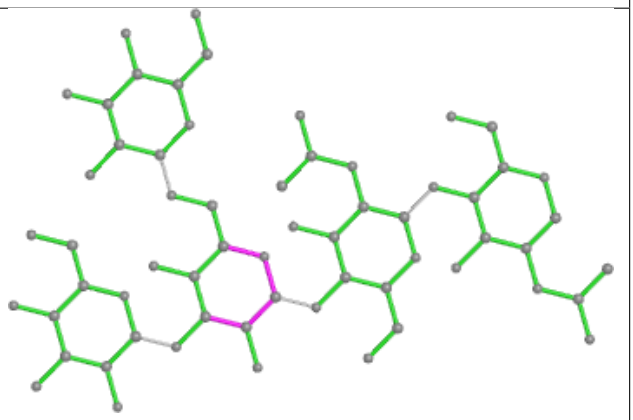


Rings

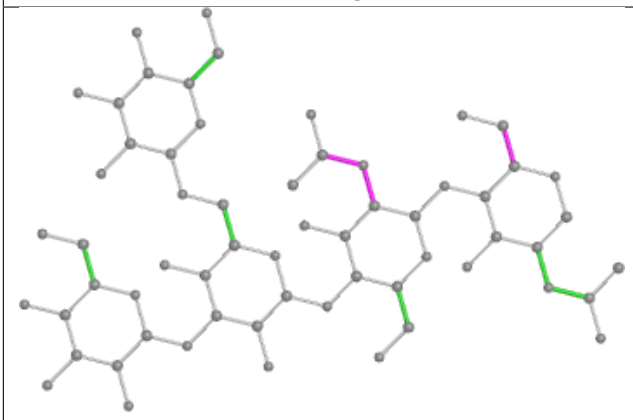
Oligosaccharide Chain E



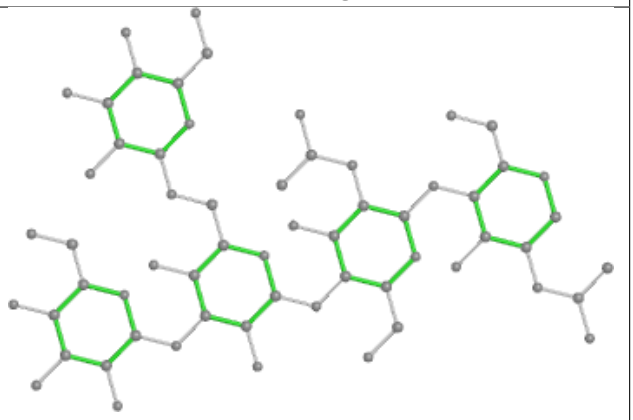
Bond lengths



Bond angles

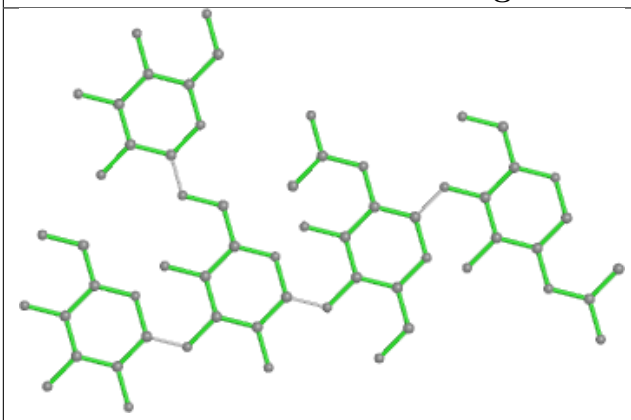


Torsions

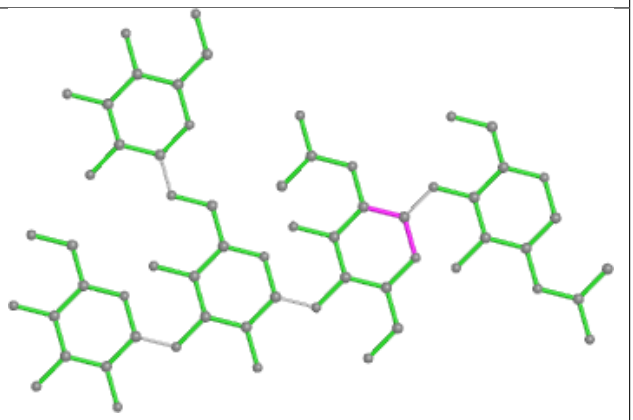


Rings

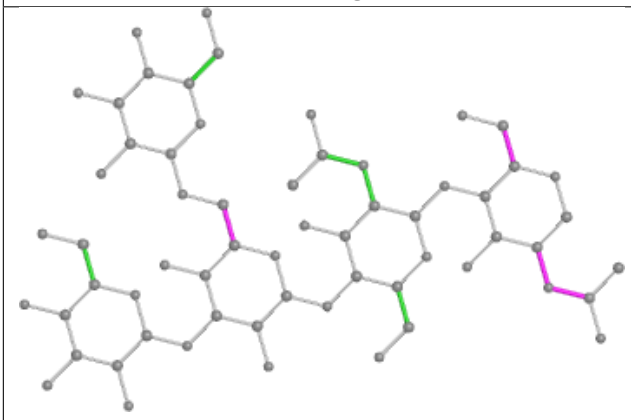
Oligosaccharide Chain H



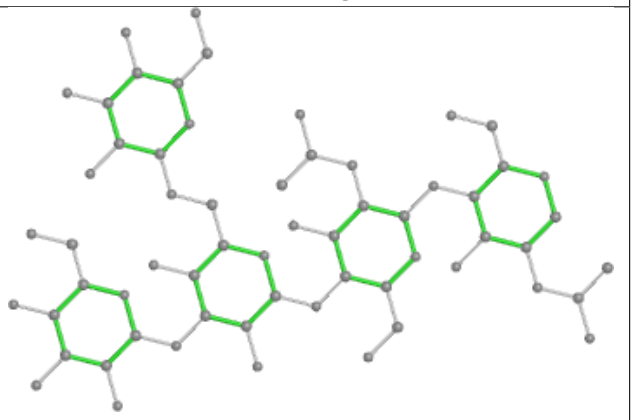
Bond lengths



Bond angles

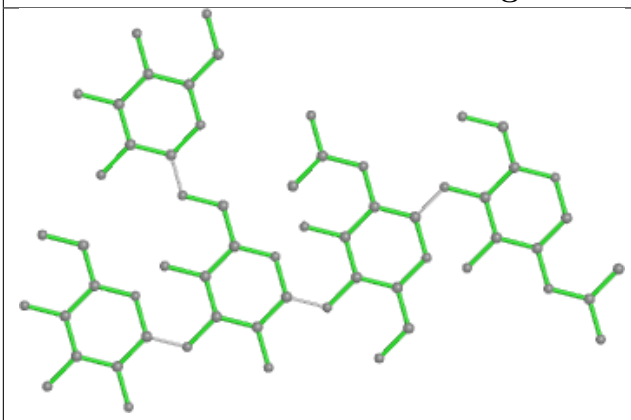


Torsions

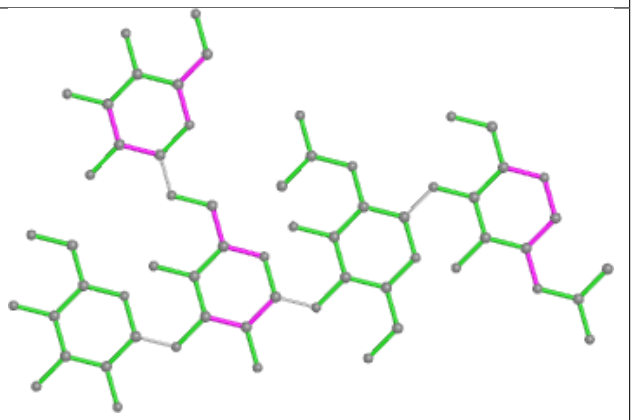


Rings

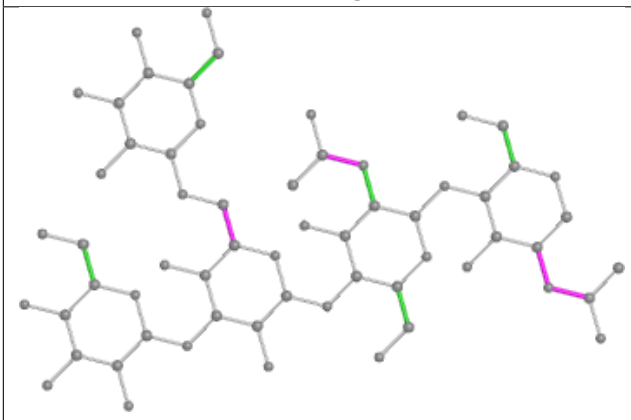
Oligosaccharide Chain I



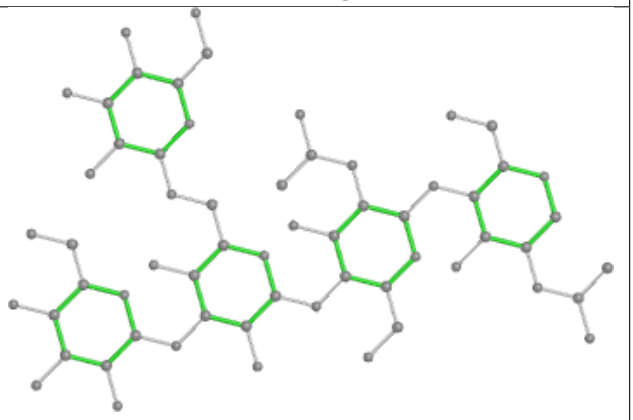
Bond lengths



Bond angles

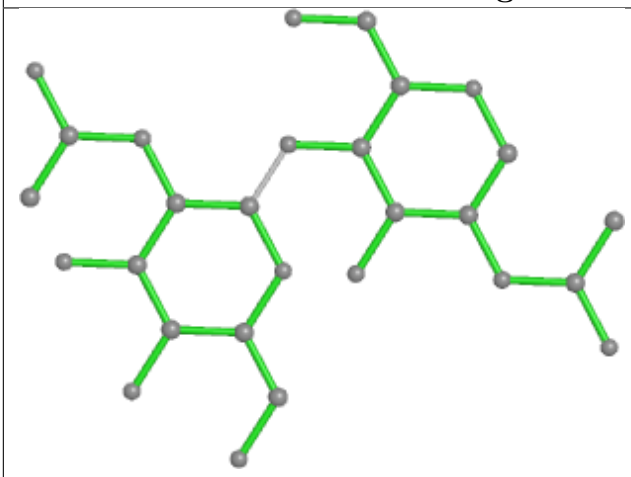


Torsions

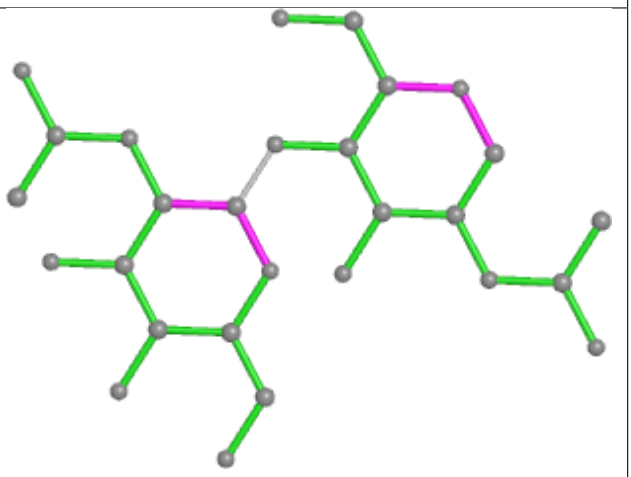


Rings

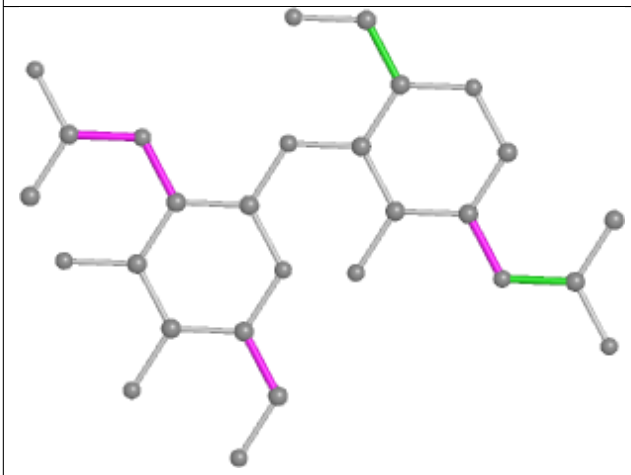
Oligosaccharide Chain F



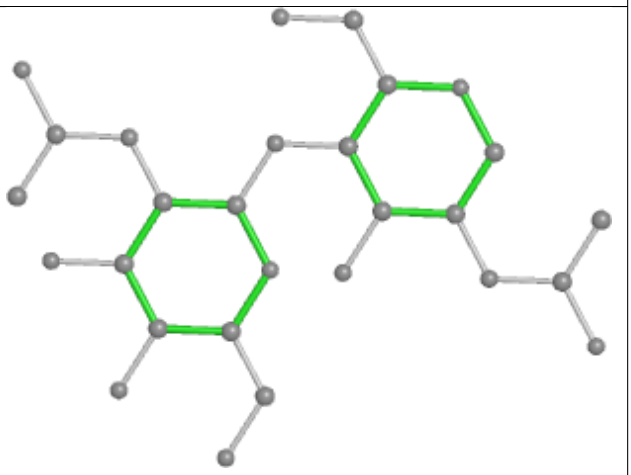
Bond lengths



Bond angles

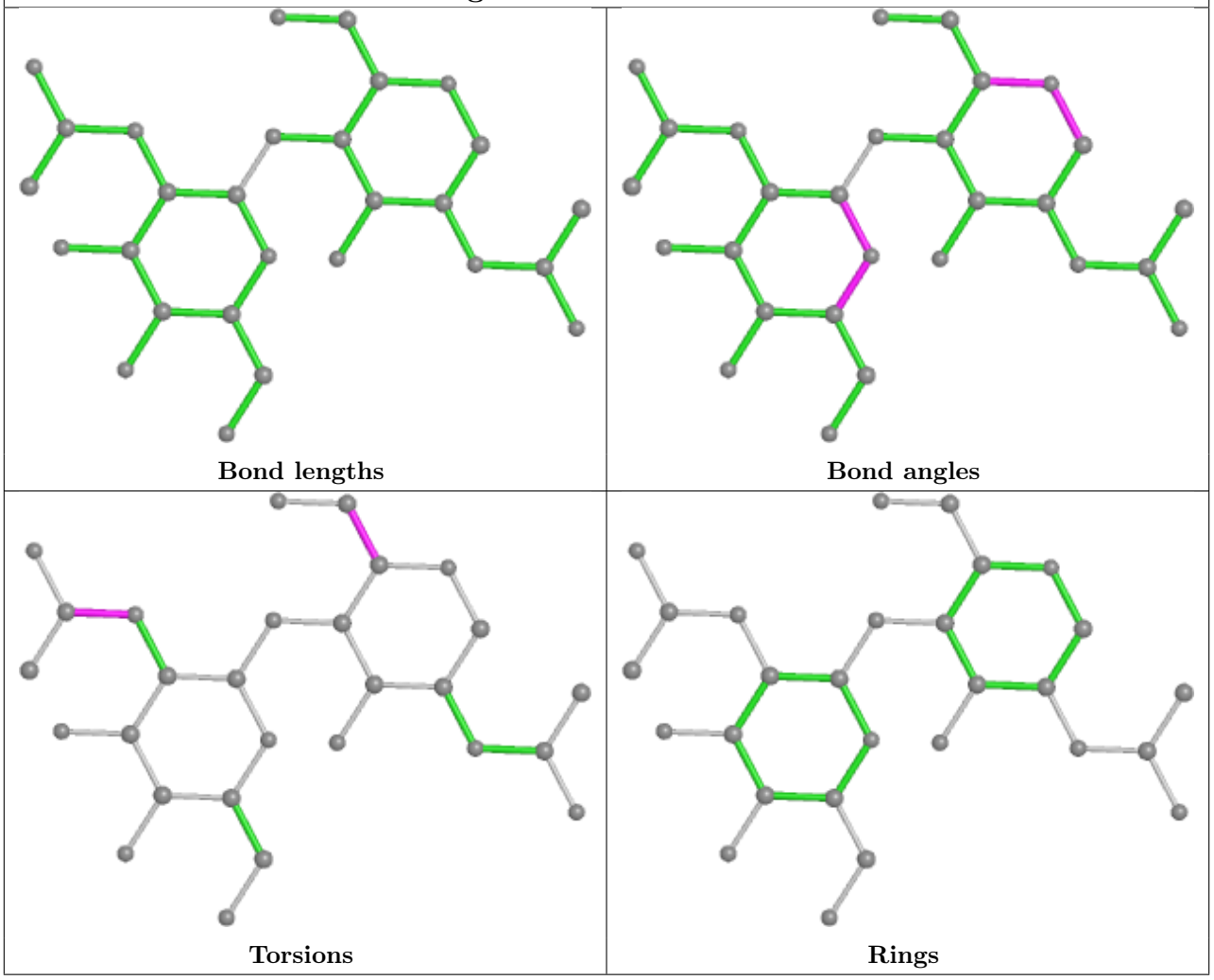


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	NAG	B	4702	1	14,14,15	0.33	0	17,19,21	0.74	1 (5%)
7	A2G	B	4705	1	14,14,15	0.42	0	17,19,21	0.67	1 (5%)
7	A2G	B	4707	1	14,14,15	0.40	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	4701	1	14,14,15	0.39	0	17,19,21	1.18	1 (5%)
7	A2G	B	4704	1	14,14,15	0.41	0	17,19,21	0.62	1 (5%)
7	A2G	B	4706	-	14,14,15	0.40	0	17,19,21	2.18	3 (17%)
7	A2G	B	4703	-	14,14,15	0.42	0	17,19,21	1.50	3 (17%)

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
6	NAG	B	4702	1	-	1/6/23/26	0/1/1/1
7	A2G	B	4705	1	-	0/6/23/26	0/1/1/1
7	A2G	B	4707	1	-	0/6/23/26	0/1/1/1
6	NAG	B	4701	1	-	4/6/23/26	0/1/1/1
7	A2G	B	4704	1	-	1/6/23/26	0/1/1/1
7	A2G	B	4706	-	-	0/6/23/26	0/1/1/1
7	A2G	B	4703	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	4706	A2G	O5-C1-C2	7.90	123.76	111.29
7	B	4703	A2G	C1-C2-N2	4.68	118.48	110.49
6	B	4701	NAG	C1-O5-C5	3.70	117.20	112.19
7	B	4706	A2G	C1-O5-C5	3.50	116.93	112.19
7	B	4703	A2G	O5-C1-C2	2.88	115.83	111.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	4701	NAG	C3-C2-N2-C7
6	B	4701	NAG	O7-C7-N2-C2
6	B	4701	NAG	C8-C7-N2-C2
6	B	4702	NAG	O5-C5-C6-O6
7	B	4704	A2G	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4701	NAG	1	0
7	B	4706	A2G	5	0
7	B	4703	A2G	6	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.

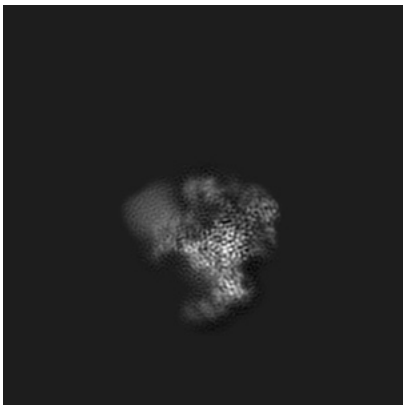
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36693. These allow visual inspection of the internal detail of the map and identification of artifacts.

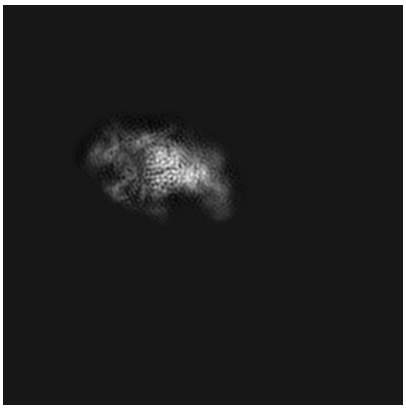
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

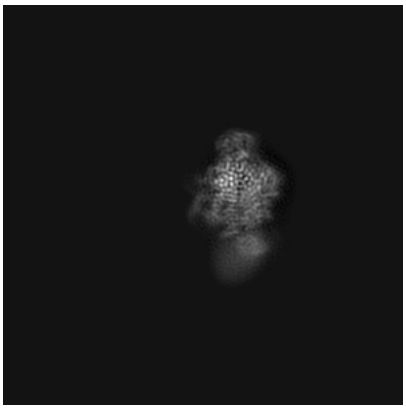
6.1.1 Primary map



X

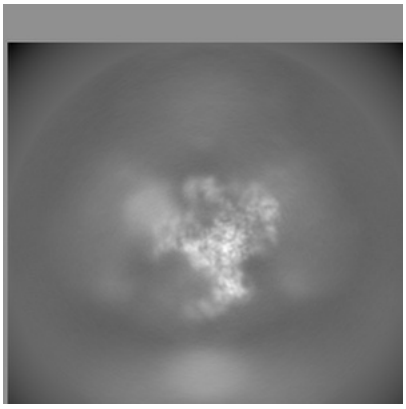


Y

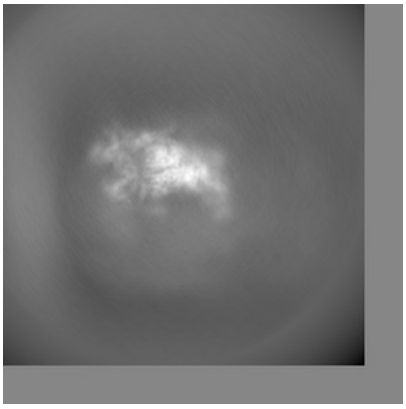


Z

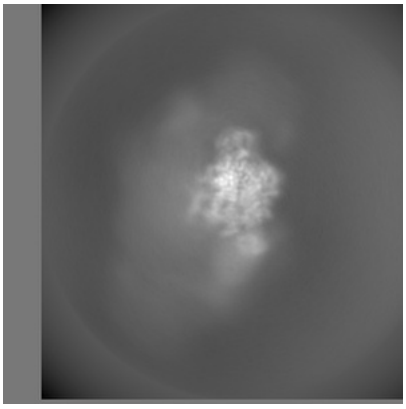
6.1.2 Raw map



X



Y

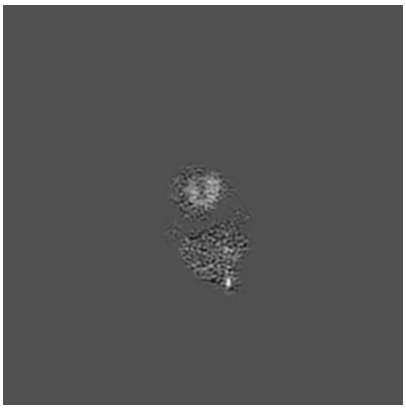


Z

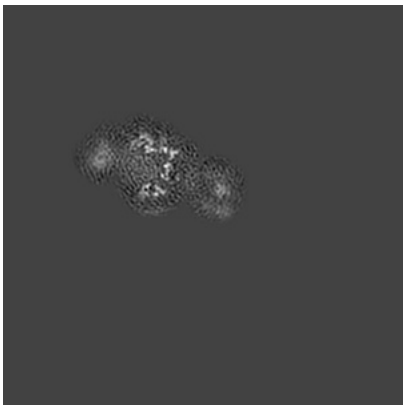
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

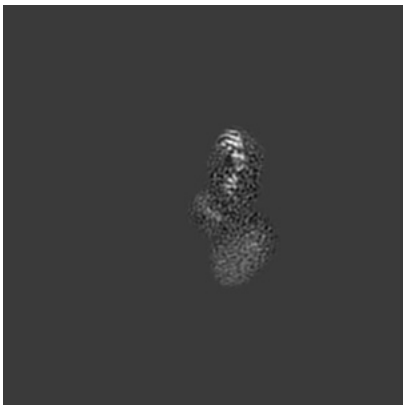
6.2.1 Primary map



X Index: 130

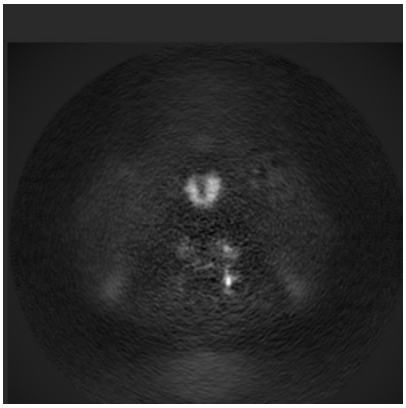


Y Index: 130

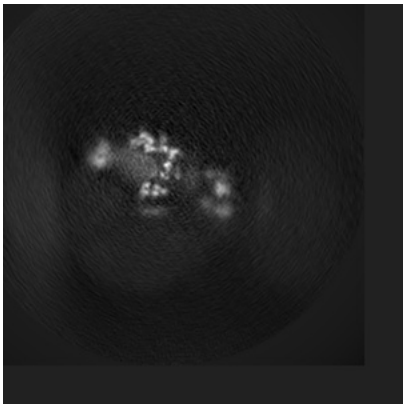


Z Index: 130

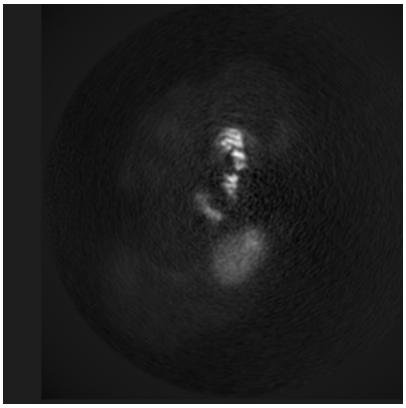
6.2.2 Raw map



X Index: 130



Y Index: 130

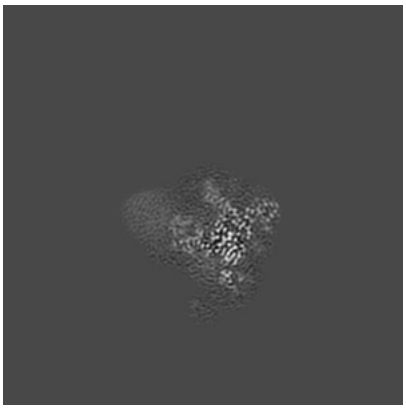


Z Index: 130

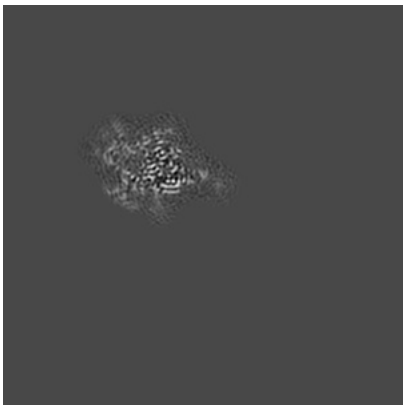
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

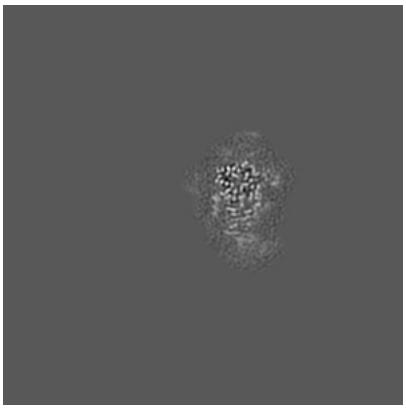
6.3.1 Primary map



X Index: 148

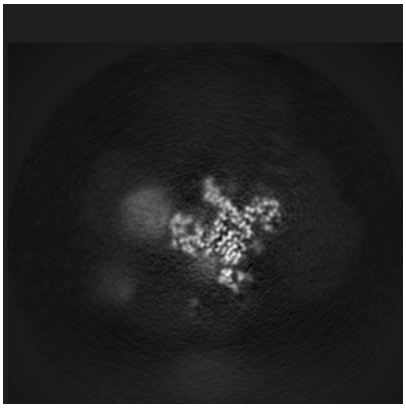


Y Index: 145

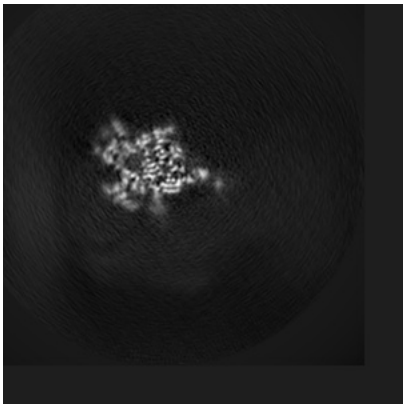


Z Index: 105

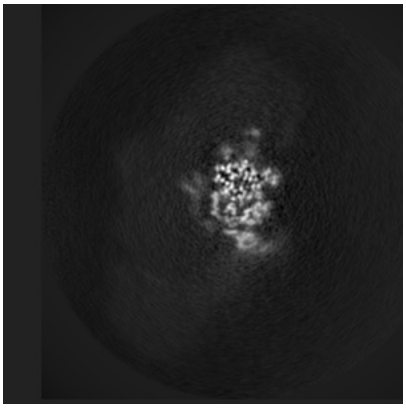
6.3.2 Raw map



X Index: 148



Y Index: 145

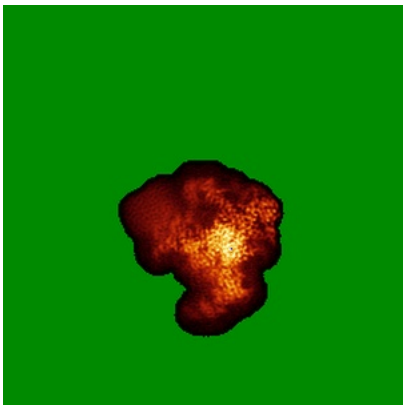


Z Index: 104

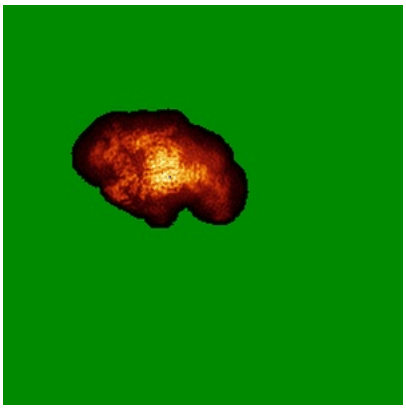
The images above show the largest variance slices of the map in three orthogonal directions.

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

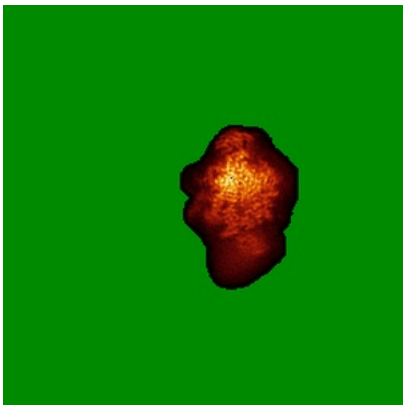
6.4.1 Primary map



X

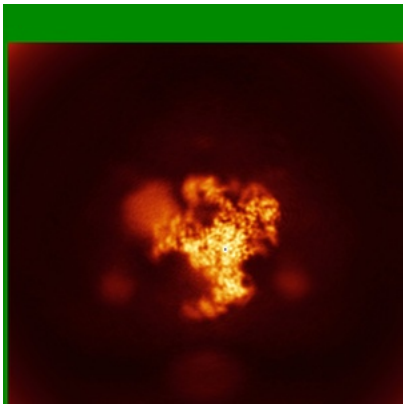


Y

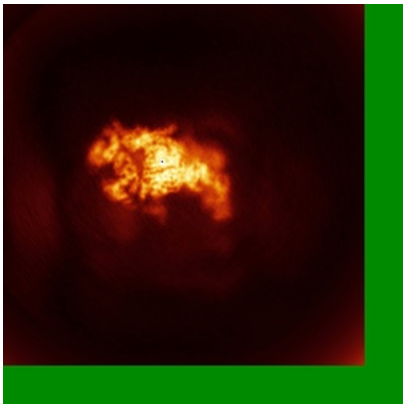


Z

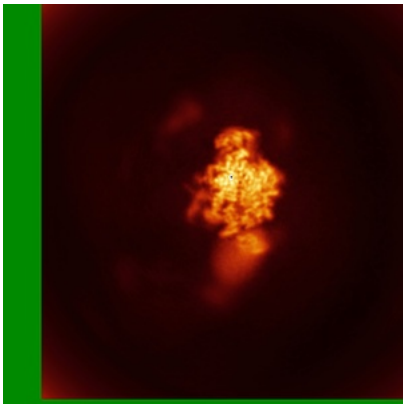
6.4.2 Raw map



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 0.035. 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.

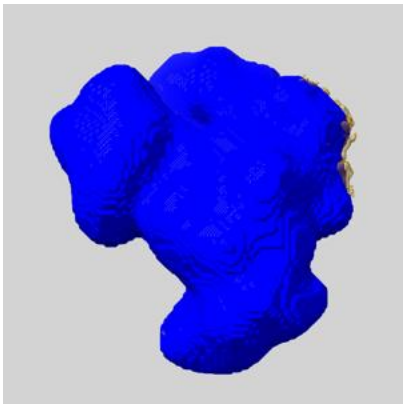
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

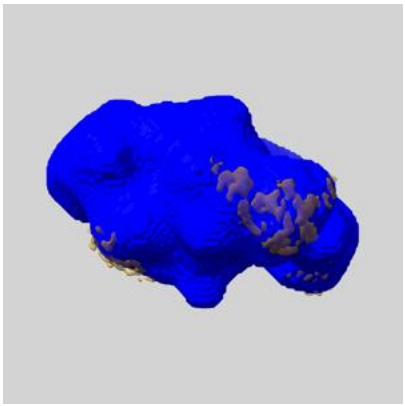
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

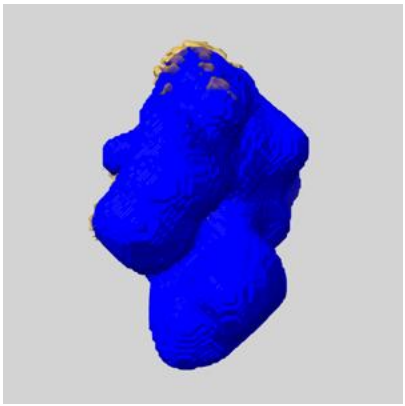
6.6.1 emd_36693_msk_1.map (i)



X



Y

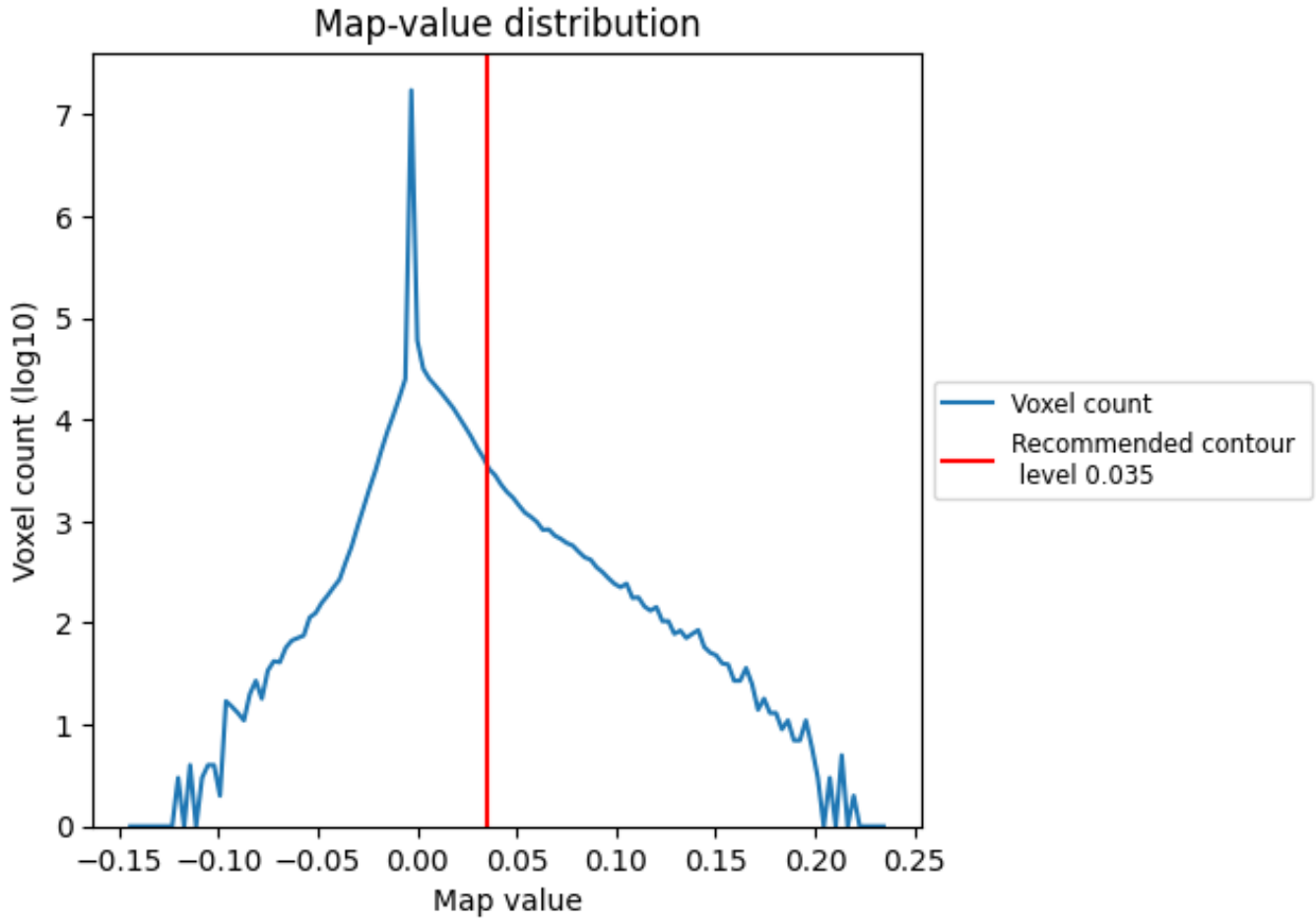


Z

7 Map analysis

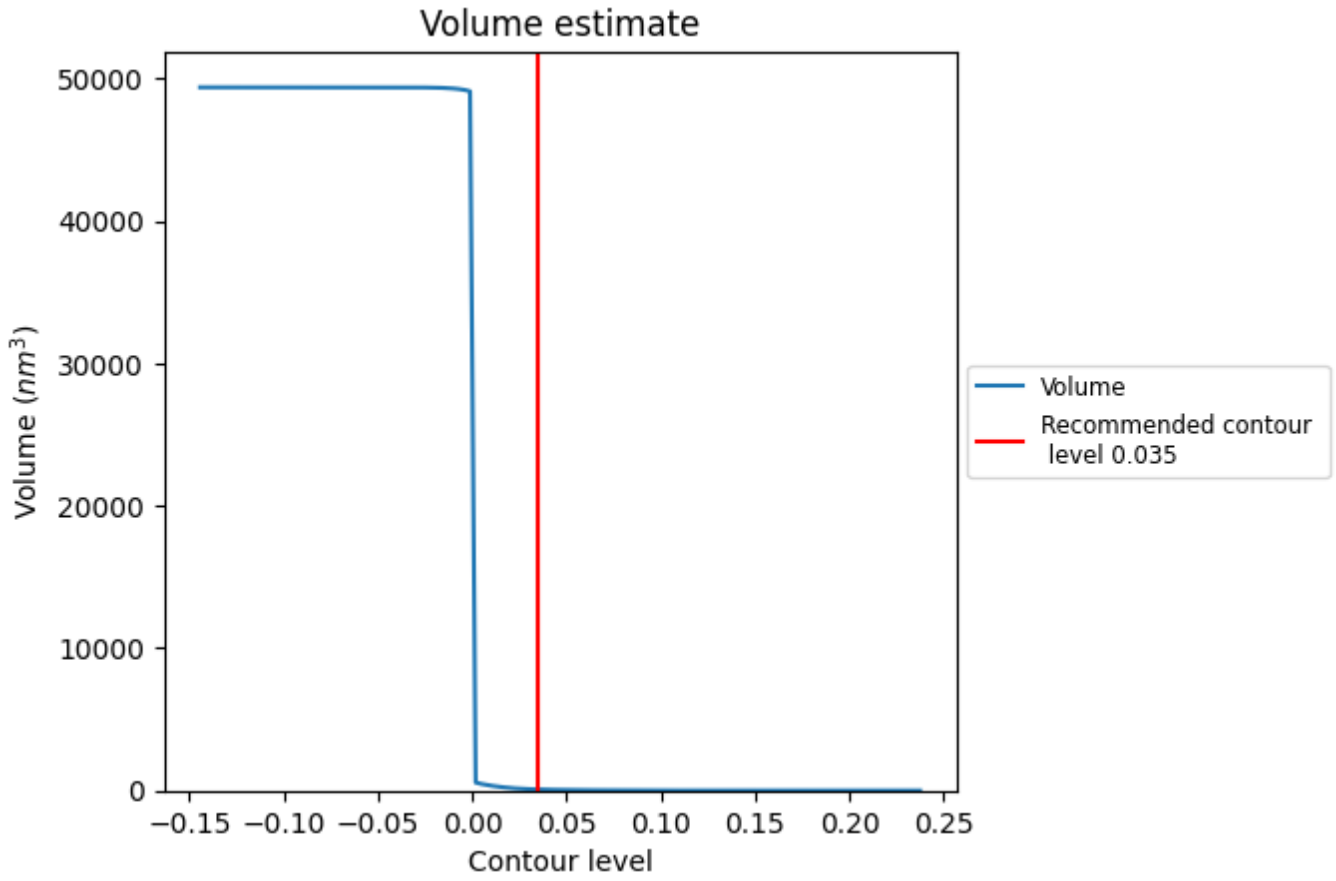
This section contains the results of statistical analysis of the map.

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.

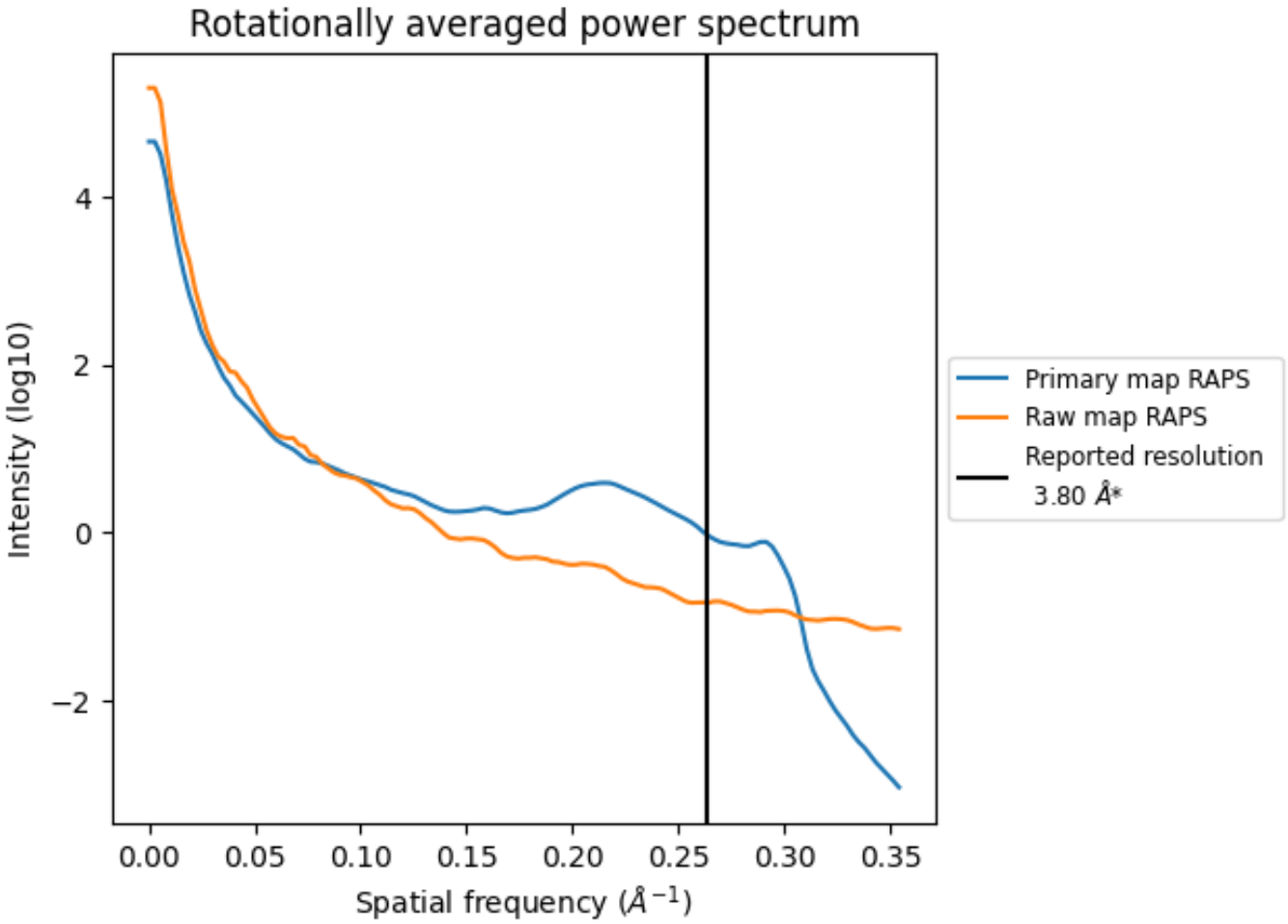
7.2 Volume estimate (i)



The volume at the recommended contour level is 77 nm^3; this corresponds to an approximate mass of 70 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)

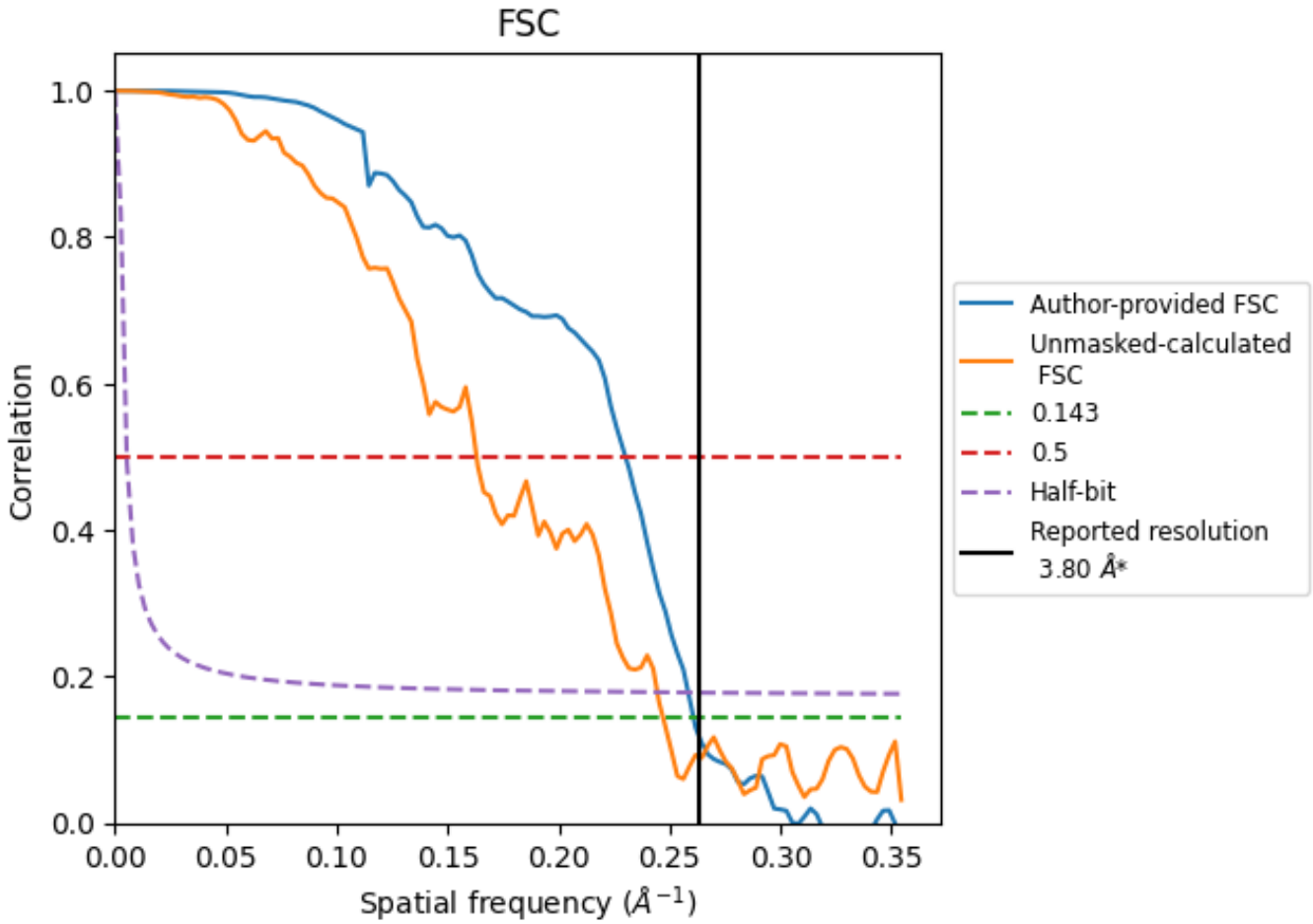


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

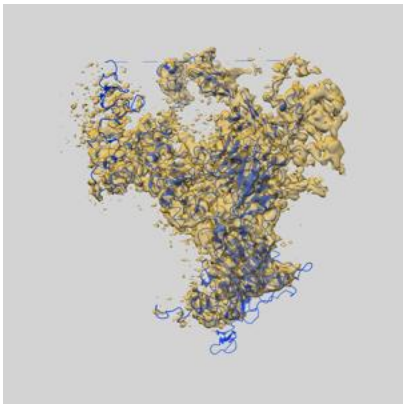
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.35	3.87
Unmasked-calculated*	4.05	6.13	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

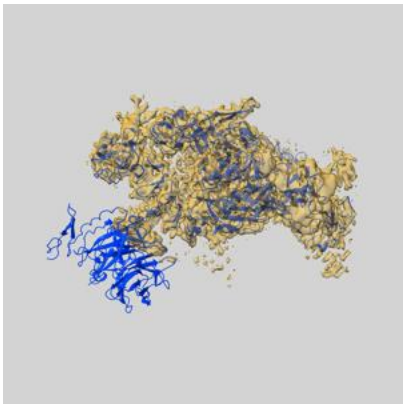
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36693 and PDB model 8JX9. Per-residue inclusion information can be found in section 3 on page 7.

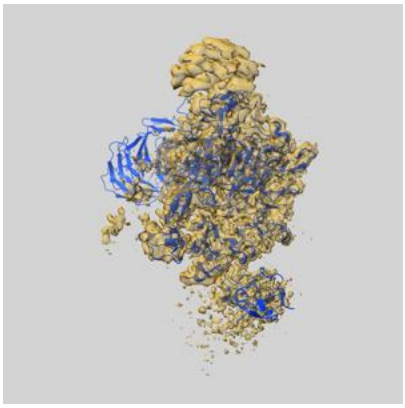
9.1 Map-model overlay



X



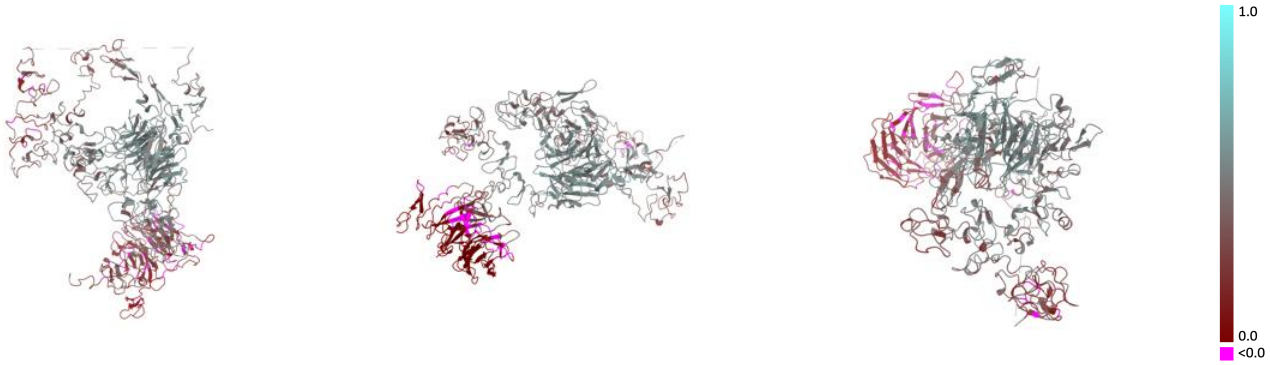
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

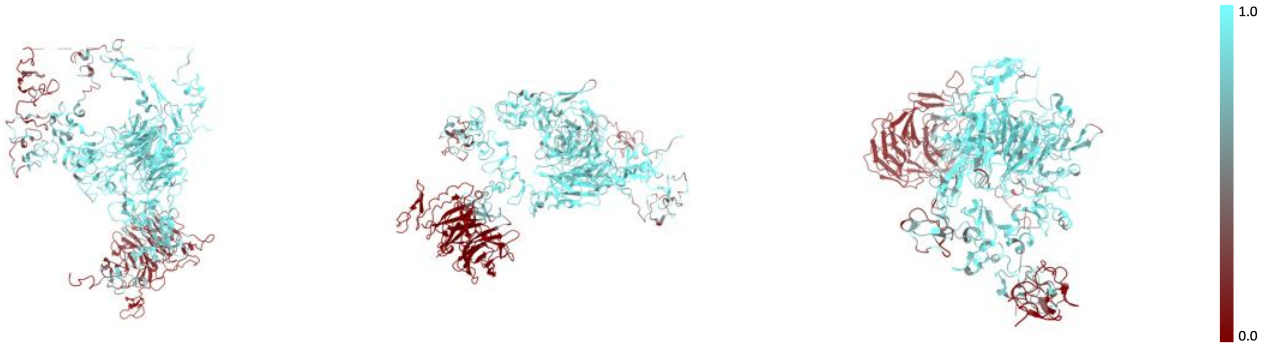
9.2 Q-score mapped to coordinate model (i)



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.

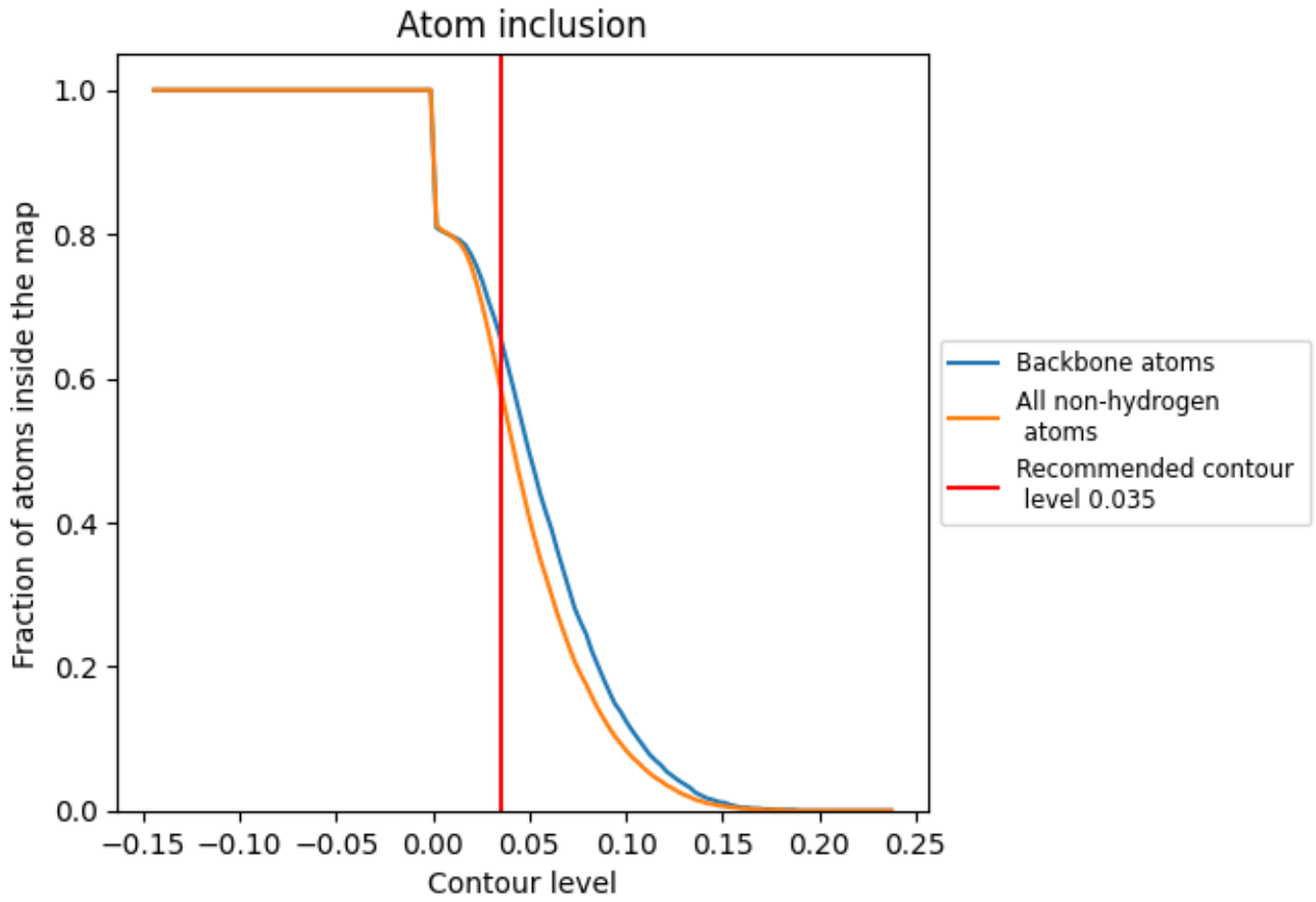
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.3480
A	0.0930	0.0690
B	0.7560	0.4390
C	0.3330	0.3370
D	0.7950	0.5070
E	0.6890	0.4650
F	0.5360	0.4360
G	0.5710	0.4210
H	0.5250	0.3520
I	0.7380	0.4320
O	1.0000	0.5960