wwPDB EM Validation Summary Report

Dec 31, 2024 – 06:15 PM EST

PDB ID	:	8JXA
EMDB ID	:	EMD-36694
Title	:	cryo-EM structure of rat megalin bodyB
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:

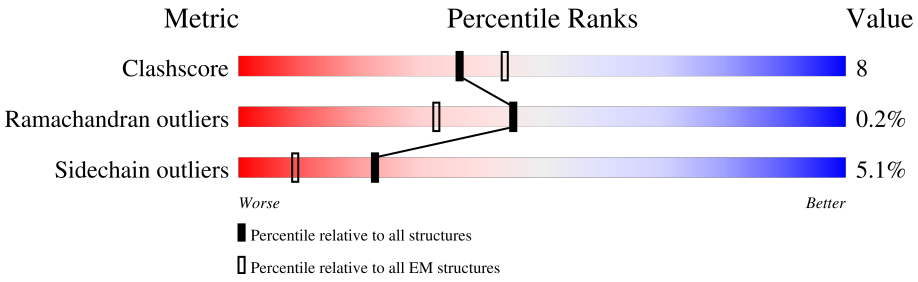
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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	5% 18% 5% 77%
1	B	4660	7% 6% 92%
2	M	5	100%
3	C	3	67% 100%
3	D	3	33% 33% 67%
4	E	5	40% 80% 20%
4	H	5	60% 80% 20%
4	I	5	20% 80% 20%

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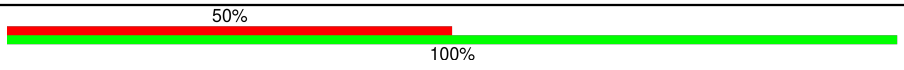
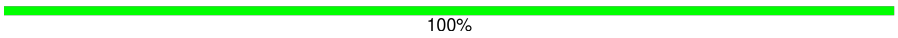
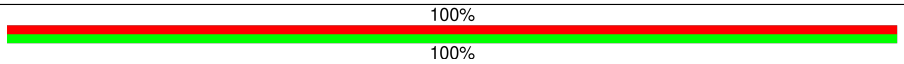
Mol	Chain	Length	Quality of chain
5	F	2	
5	G	2	
5	J	2	
6	K	3	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11889 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.

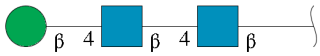
- Molecule 1 is a protein called LDL receptor related protein 2.

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

- Molecule 2 is a protein called unclear peptide.

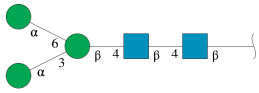
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	5	Total	C	N	O	0	0
			28	16	6	6		

- 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.

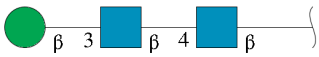


Mol	Chain	Residues	Atoms	AltConf	Trace
4	E	5	Total C N O 61 34 2 25	0	0
4	H	5	Total C N O 61 34 2 25	0	0
4	I	5	Total C N O 61 34 2 25	0	0

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

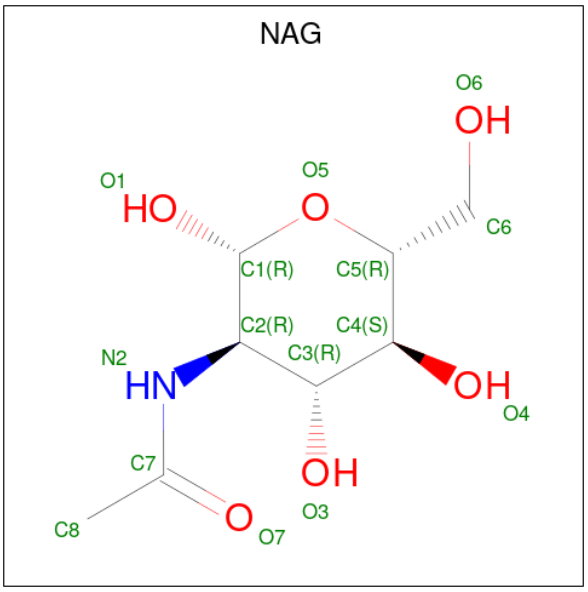
Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	2	Total C N O 28 16 2 10	0	0
5	G	2	Total C N O 28 16 2 10	0	0
5	J	2	Total C N O 28 16 2 10	0	0

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



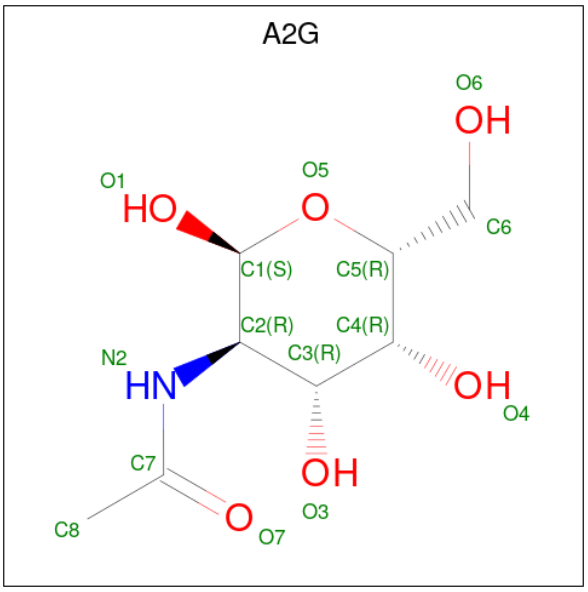
Mol	Chain	Residues	Atoms	AltConf	Trace
6	K	3	Total C N O 39 22 2 15	0	0

- 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	

- Molecule 8 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

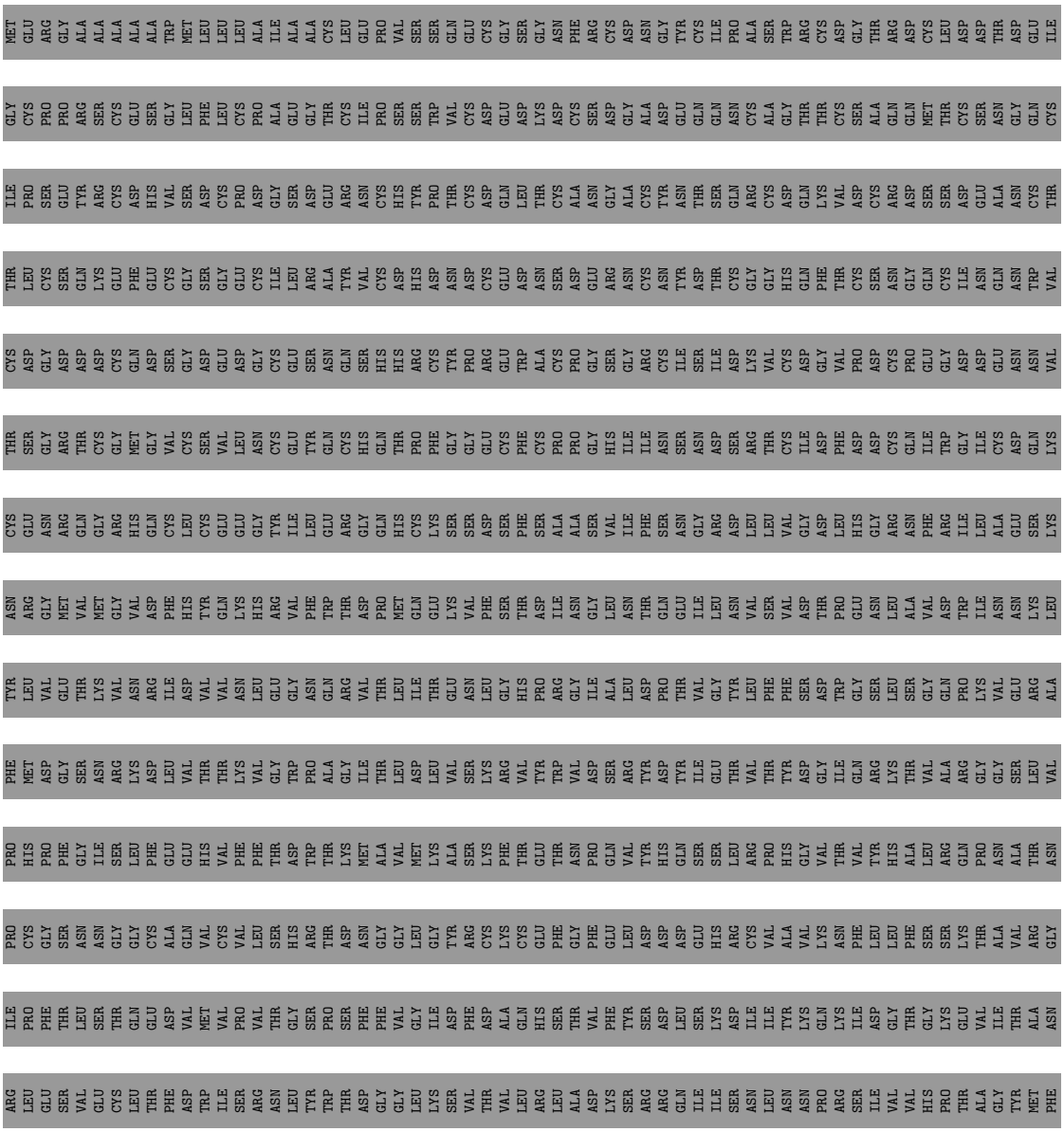
Mol	Chain	Residues	Atoms		AltConf
9	A	20	Total	Ca	0
			20	20	

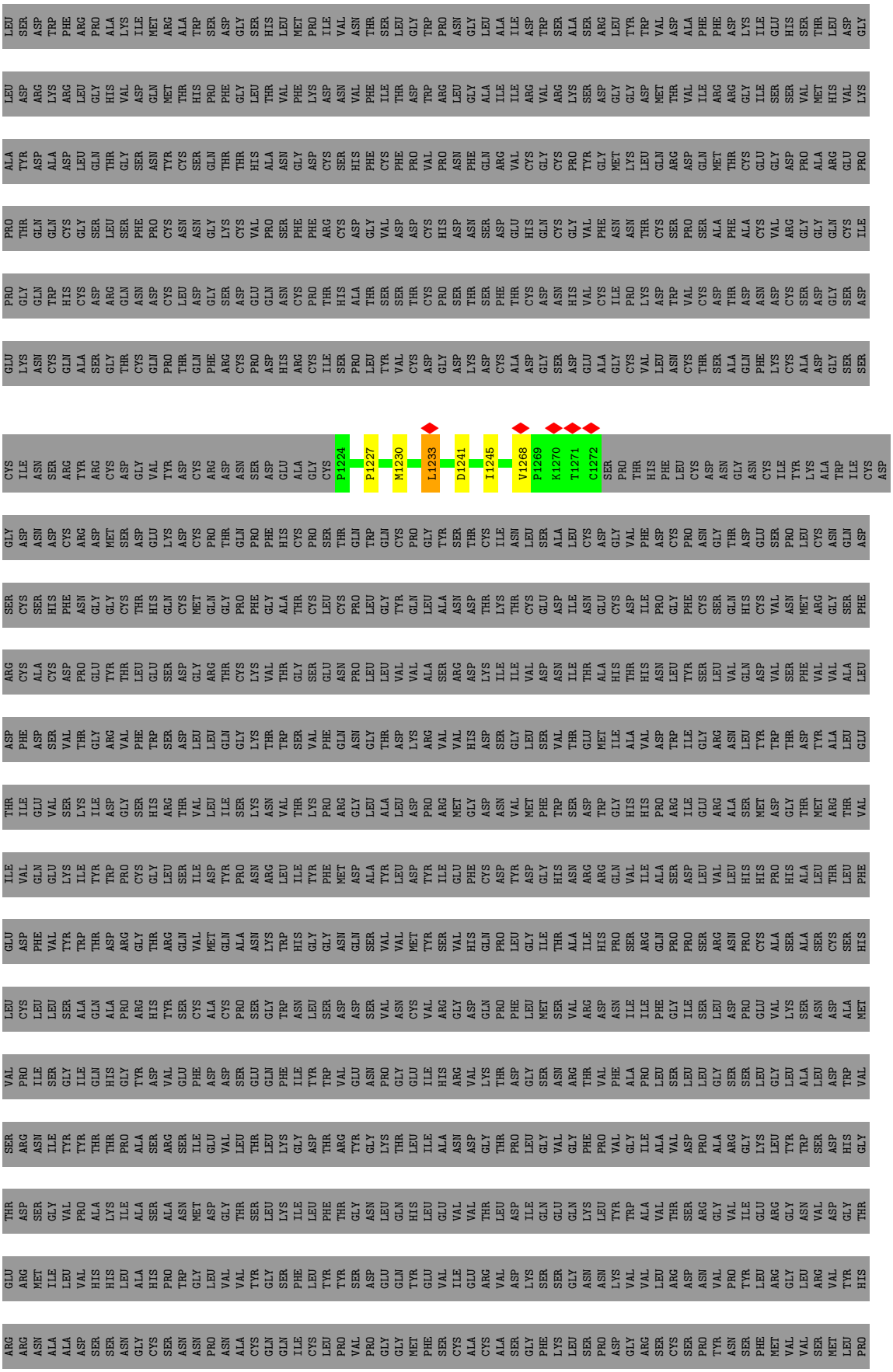
3 Residue-property plots (i)

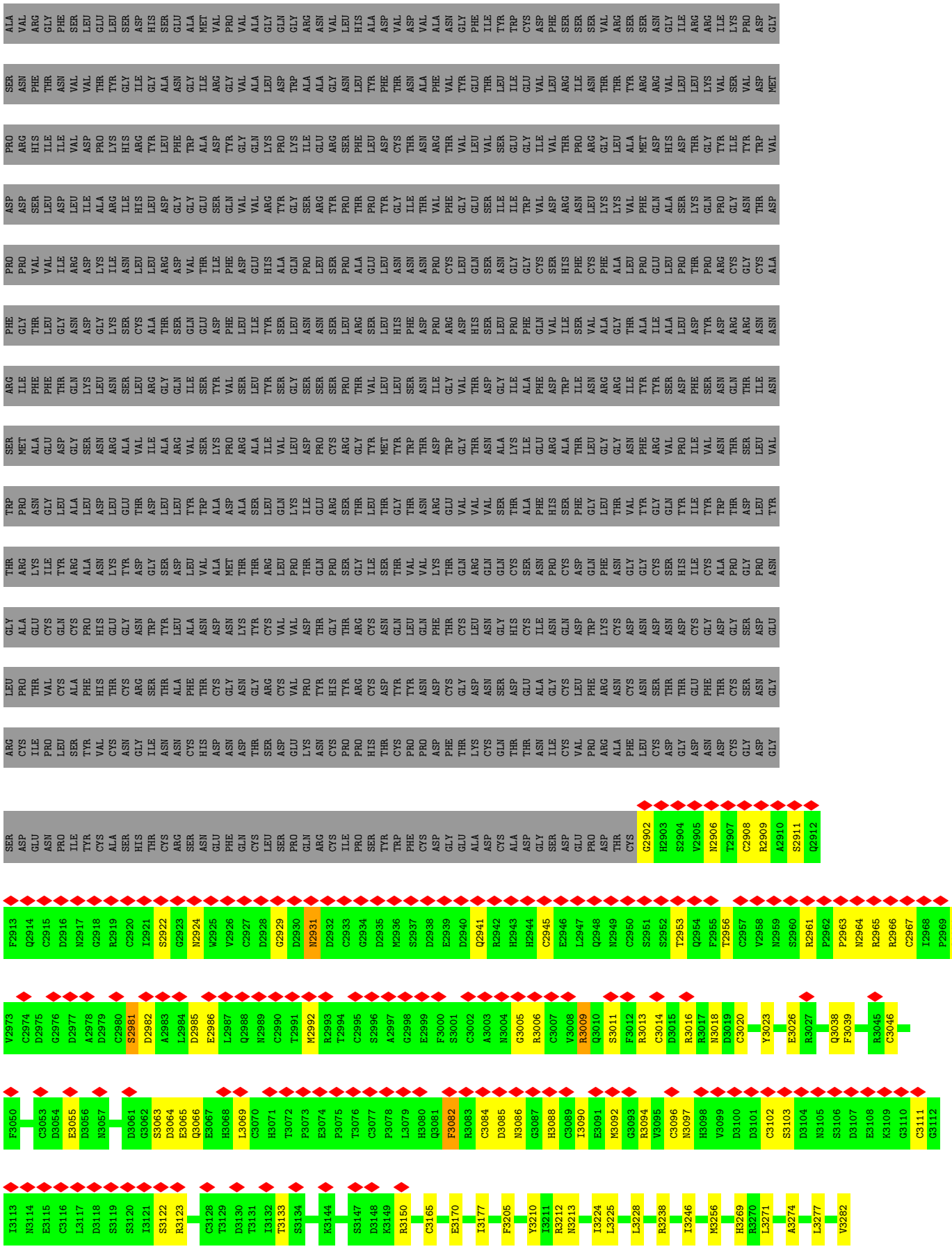
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

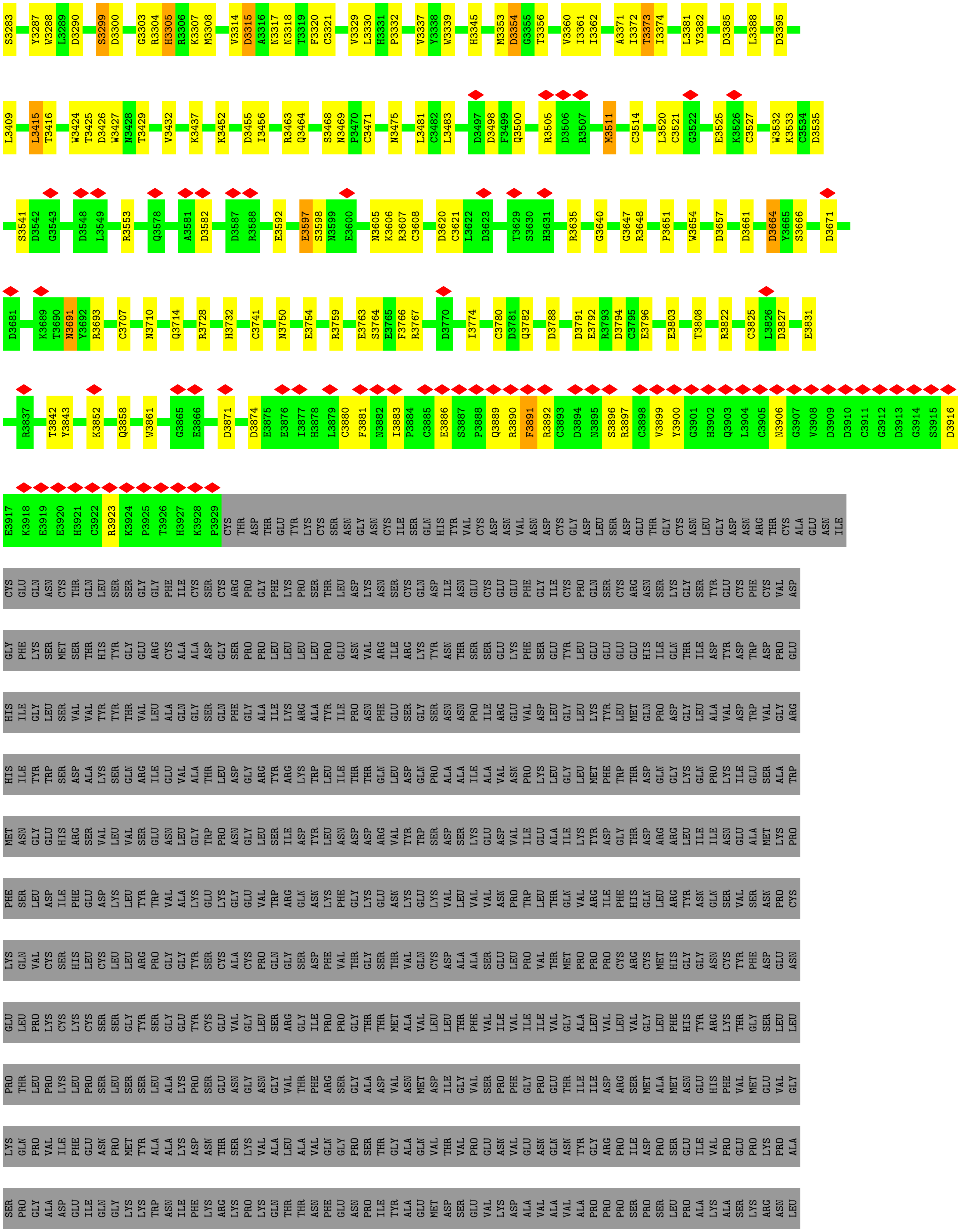
- Molecule 1: LDL receptor related protein 2

Chain A:




P1224
P1227
M1230
L1233
D1241
I1245
V1268
P1269
K1270
T1271
C1272

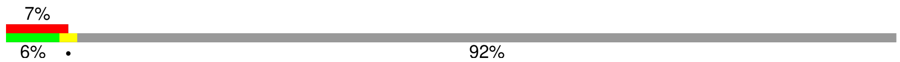




THR PRO GLY TYR THR ALA THR GLU ASP THR PHE LYS ASP THR ALA ASN LEU VAL LYS GLU ASP SER ASP VAL

- Molecule 1: LDL receptor related protein 2

Chain B:



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 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 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

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

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

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

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

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

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

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

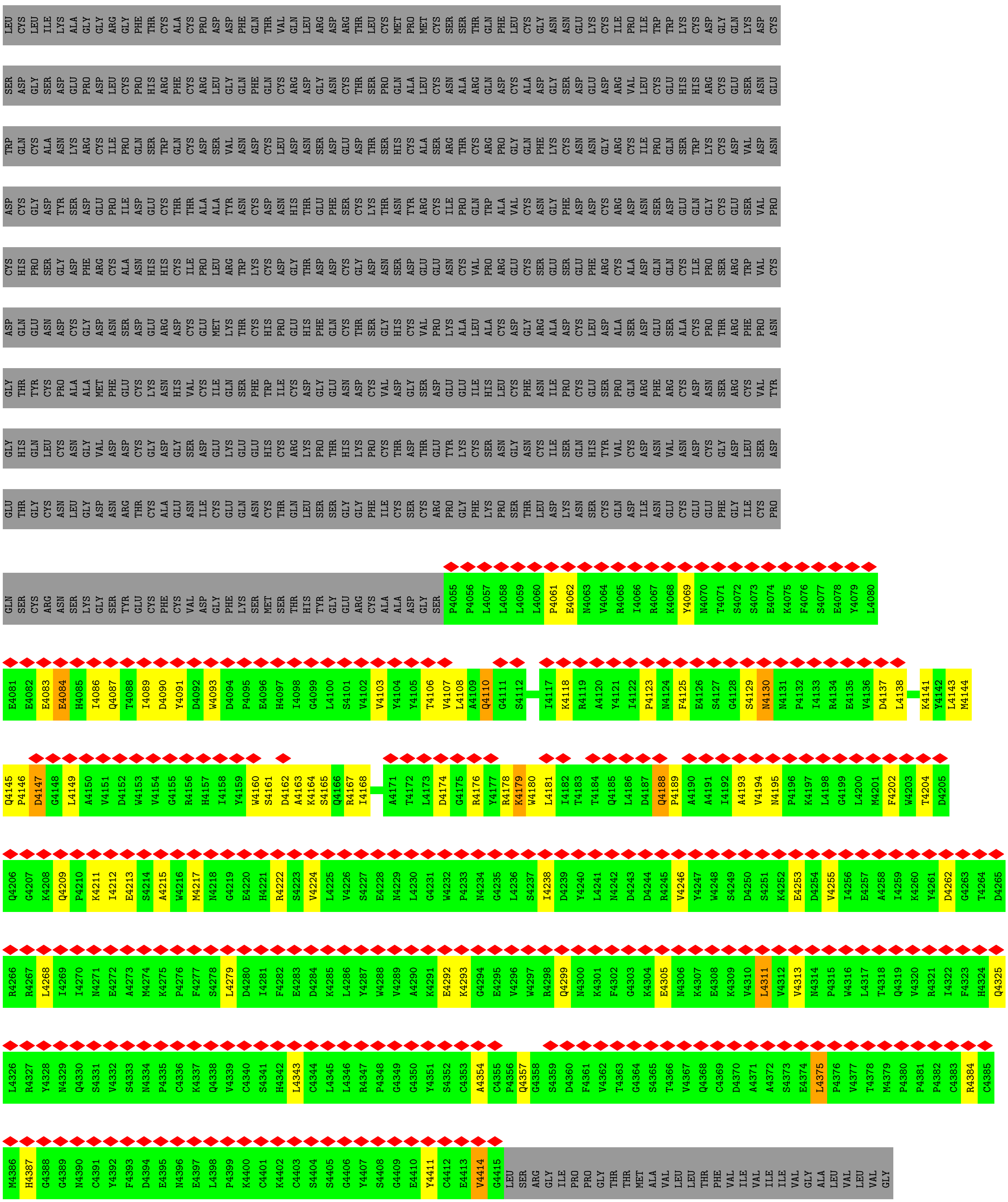
ALA PRO GLY TYR ILE ARG GLU PRO ASP GLY LYS SER CYS ARG GLN ASN SER ASN ILE GLU PRO TYR LEU ILE PHE SER ASN ARG TYR TYR ILE ARG ASN LEU THR THR ASP GLY SER SER TYR SER LEU ILE LEU GLN GLY LEU GLY ASN VAL VAL ALA LEU ASP PHE ASP ARG VAL GLU

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

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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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
ASP CYS GLY ASP TYR SER ASP GLU PRO ILE ASP GLU CYS THR THR ALA ALA TYR ASN CYS ASP ASN HIS THR GLU PHE SER CYS LYS THR ASN TYR ARG CYS ILE PRO GLN TRP ALA VAL CYS ASN GLY PHE ASP ASP CYS ARG ASP ASN SER ASP GLU GLN GLY CYS GLU SER VAL PRO
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 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 A4109 Q4110 G4111 S4112 I4117 K4118 R4119 A4120 Y4121 I4122 P4123 N4124 F4125 E4126 S4127 G4128 S4129 N4130 N4131 P4132 I4133 R4134 E4135 V4136 D4137 L4138 K4141 Y4142 L4143 M4144
Q4145 P4146 D4147 G4148 L4149 A4150 V4151 D4152 W4153 V4154 G4155 R4156 H4157 I4158 Y4159 W4160 S4161 D4162 A4163 K4164 S4165 Q4166 R4167 I4168 A4171 T4172 L4173 D4174 G4175 R4176 Y4177 R4178 K4179 W4180 L4181 I4182 T4183 T4184 Q4185 L4186 D4187 Q4188 P4189 A4190 A4191 I4192 A4193 V4194 N4195 P4196 K4197 L4198 G4199 L4200 M4201 F4202 W4203 T4204 D4205
Q4206 G4207 K4208 Q4209 P4210 K4211 I4212 E4213 S4214 A4215 W4216 M4217 N4218 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 V4339 C4340 S4341 H4342 L4343 C4344 L4345 L4346 R4347 P4348 G4349 G4350 Y4351 S4352 C4353 A4354 C4355 P4356 Q4357 G4358 S4359 D4360 F4361 V4362 T4363 G4364 S4365 T4366 V4367 Q4368 C4369 D4370 A4371 A4372 S4373 E4374 L4375 P4376 V4377 T4378 M4379 P4380 P4381 P4382 C4383 R4384 C4385
M4386 H4387 G4388 G4389 N4390 C4391 Y4392 F4393 D4394 E4395 N4396 E4397 L4398 P4399 K4400 C4401 K4402 C4403 S4404 S4405 G4406 Y4407 S4408 G4409 E4410 Y4411 C4412 E4413 V4414 G4415 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

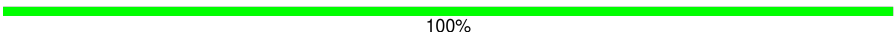
ALA MET ASN GLU HIS PHE VAL MET GLU VAL GLY LYS GLN PRO VAL ILE PHE GLU ASN PRO MET TYR ALA ALA LYS ASP ASN THR SER LYS VAL ALA LEU ALA VAL GLN GLY PRO SER THR GLY ALA GLN VAL THR VAL PRO GLU ASN VAL GLU ASN GLN ASN TYR GLY ARG PRO ILE ASP

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

• Molecule 2: unclear peptide

Chain M:



There are no outlier residues recorded for this chain.

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

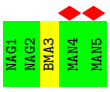
Chain C:

• 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:

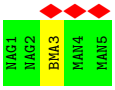
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



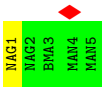
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



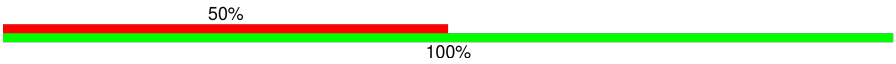
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

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

Chain J:

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

Chain K:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0434	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: A2G, CA, BMA, MAN, NAG

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	0.28	0/8659	0.54	0/11737
1	B	0.24	0/2981	0.50	0/4047
2	M	0.14	0/7	0.28	0/8
All	All	0.27	0/11647	0.53	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	8455	0	7527	128	0
1	B	2904	0	2797	42	0
2	M	28	0	12	0	0
3	C	39	0	34	0	0
3	D	39	0	34	1	0
4	E	61	0	52	0	0
4	H	61	0	52	0	0
4	I	61	0	52	0	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
5	J	28	0	25	0	0
6	K	39	0	34	0	0
7	A	28	0	26	0	0
8	A	70	0	60	0	0
9	A	20	0	0	0	0
All	All	11889	0	10755	170	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 8.

The worst 5 of 170 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:4179:LYS:HA	1:B:4357:GLN:HB2	1.66	0.76
1:B:4086:ILE:HG22	1:B:4107:VAL:HG12	1.74	0.70
1:A:3238:ARG:NH1	1:A:3464:GLN:O	2.26	0.69
1:A:3092:MET:SD	1:A:3092:MET:N	2.67	0.66
1:B:4129:SER:O	1:B:4130:ASN:ND2	2.28	0.66

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	1073/4660 (23%)	984 (92%)	87 (8%)	2 (0%)	44 74
1	B	359/4660 (8%)	332 (92%)	26 (7%)	1 (0%)	37 69
2	M	1/5 (20%)	1 (100%)	0	0	100 100
All	All	1433/9325 (15%)	1317 (92%)	113 (8%)	3 (0%)	45 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3315	ASP
1	B	4414	VAL
1	A	3305	HIS

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	965/4089 (24%)	923 (96%)	42 (4%)	24 48
1	B	320/4089 (8%)	297 (93%)	23 (7%)	12 36
2	M	1/1 (100%)	1 (100%)	0	100 100
All	All	1286/8179 (16%)	1221 (95%)	65 (5%)	22 45

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4246	VAL
1	B	4279	LEU
1	A	3505	ARG
1	A	3468	SER
1	B	4311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4387	HIS
1	B	4145	GLN
1	A	3714	GLN
1	A	3679	ASN
1	A	3782	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)

30 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	0.33	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.64	0
3	BMA	C	3	3	11,11,12	0.25	0	15,15,17	0.64	0
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.49	0
4	NAG	E	1	1,4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.69	0
4	BMA	E	3	4	11,11,12	0.27	0	15,15,17	0.91	1 (6%)
4	MAN	E	4	4	11,11,12	0.25	0	15,15,17	0.60	0
4	MAN	E	5	4	11,11,12	0.21	0	15,15,17	0.59	0
5	NAG	F	1	1,5	14,14,15	0.27	0	17,19,21	0.70	0
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	0.55	0
5	NAG	G	1	1,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	H	1	1,4	14,14,15	0.32	0	17,19,21	0.89	0
4	NAG	H	2	4	14,14,15	0.32	0	17,19,21	0.59	0
4	BMA	H	3	4	11,11,12	0.24	0	15,15,17	0.85	1 (6%)
4	MAN	H	4	4	11,11,12	0.22	0	15,15,17	0.54	0
4	MAN	H	5	4	11,11,12	0.22	0	15,15,17	0.60	0
4	NAG	I	1	1,4	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.70	0
4	BMA	I	3	4	11,11,12	0.23	0	15,15,17	0.74	0
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.55	0
4	MAN	I	5	4	11,11,12	0.22	0	15,15,17	0.53	0
5	NAG	J	1	5	14,14,15	0.28	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	J	2	5	14,14,15	0.32	0	17,19,21	0.69	0
6	NAG	K	1	6	14,14,15	0.27	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.32	0	17,19,21	0.60	0
6	BMA	K	3	6	11,11,12	0.23	0	15,15,17	0.66	0

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	C1-O5-C5	2.50	115.54	112.19
4	H	3	BMA	C1-O5-C5	2.36	115.34	112.19
3	D	1	NAG	C2-N2-C7	-2.25	119.88	122.90
4	E	3	BMA	C1-C2-C3	2.12	112.72	109.64
3	D	2	NAG	C2-N2-C7	-2.04	120.16	122.90

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
6	K	3	BMA	O5-C5-C6-O6

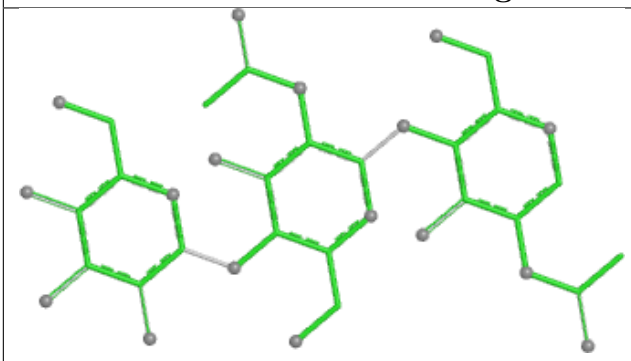
There are no ring outliers.

2 monomers are involved in 1 short contact:

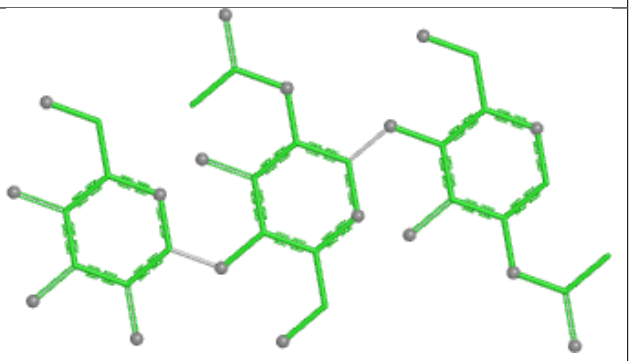
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	D	2	NAG	1	0

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

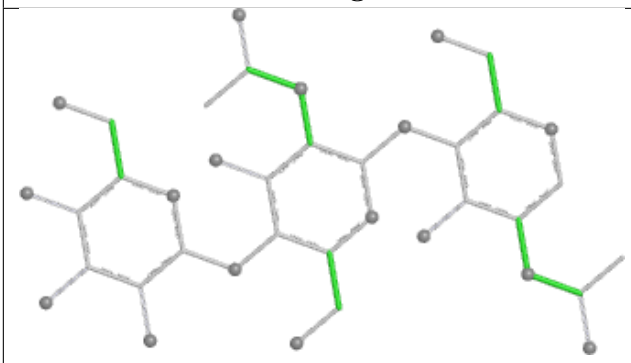
Oligosaccharide Chain C



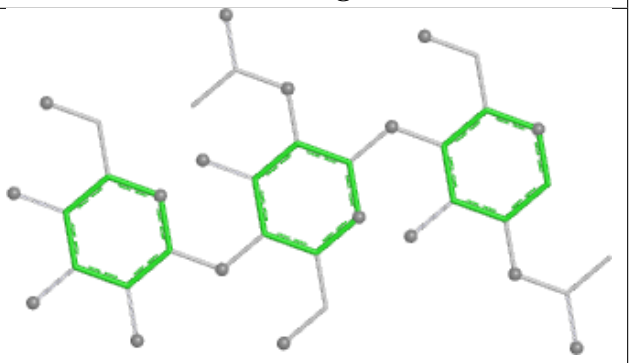
Bond lengths



Bond angles

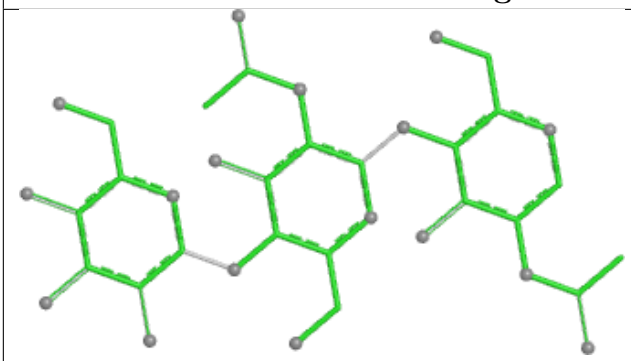


Torsions

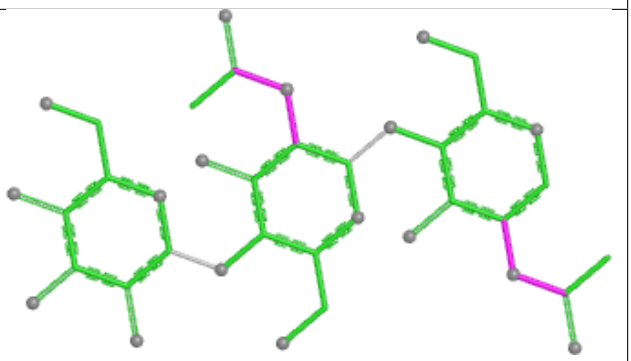


Rings

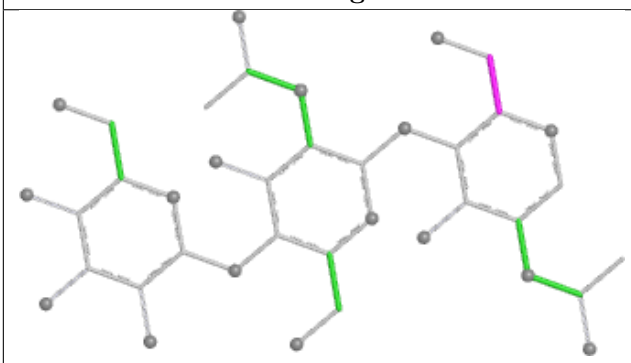
Oligosaccharide Chain D



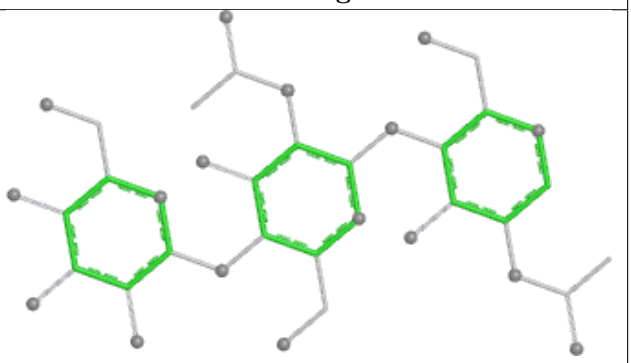
Bond lengths



Bond angles

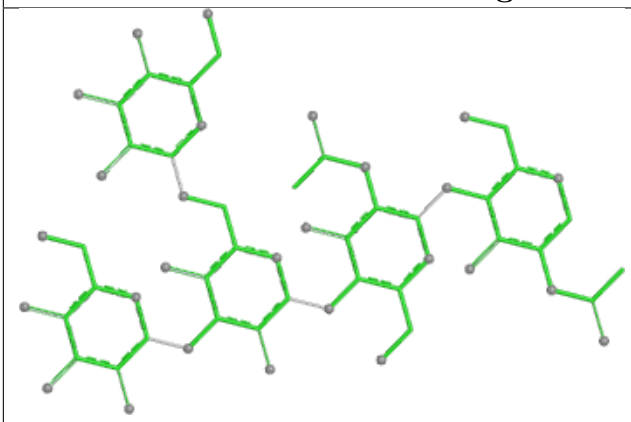


Torsions

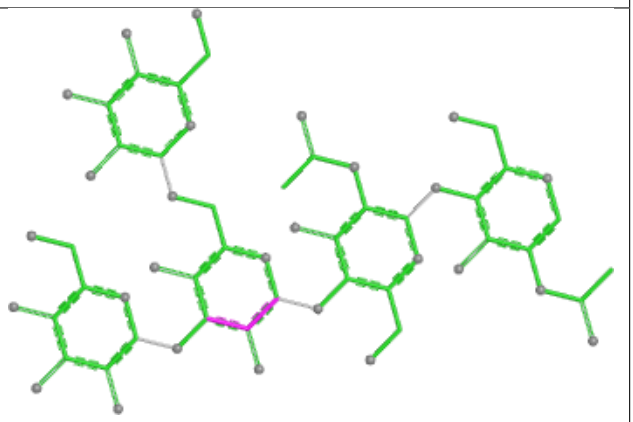


Rings

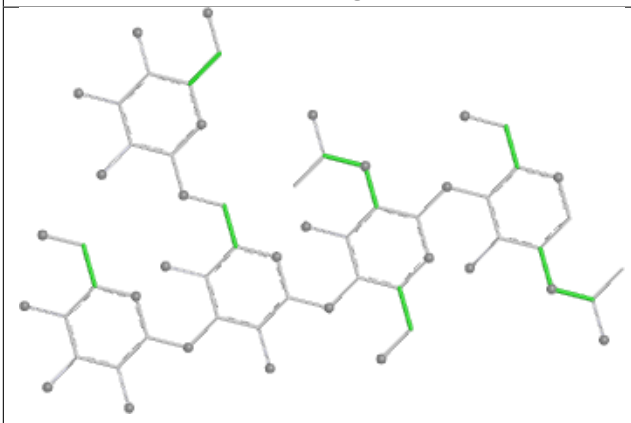
Oligosaccharide Chain E



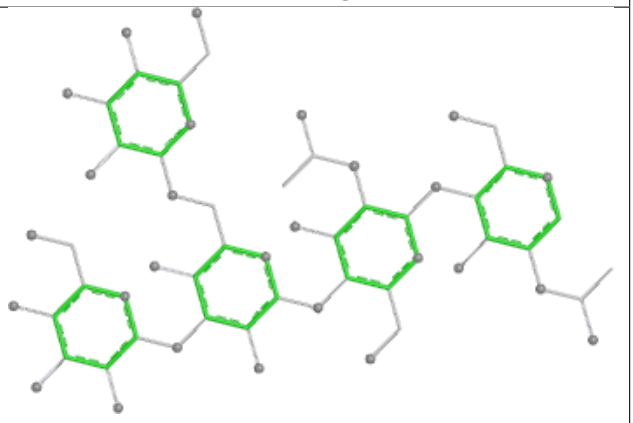
Bond lengths



Bond angles

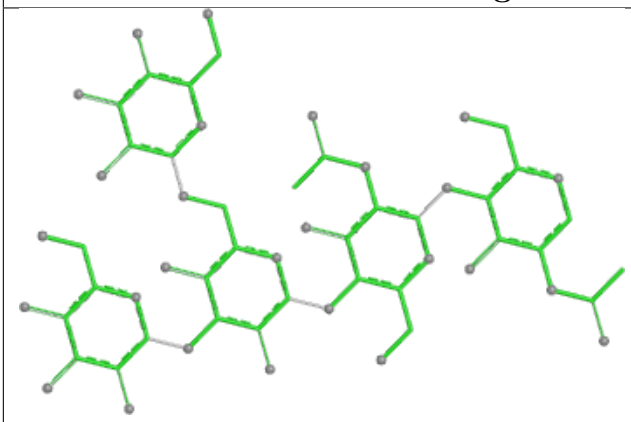


Torsions

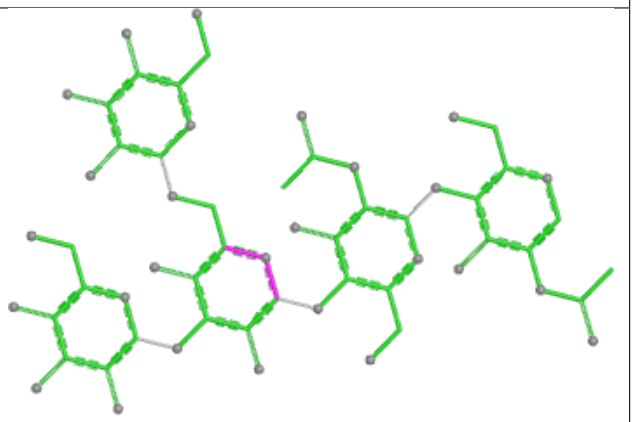


Rings

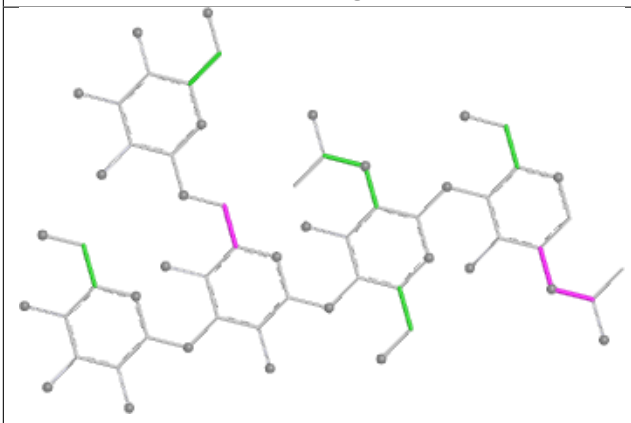
Oligosaccharide Chain H



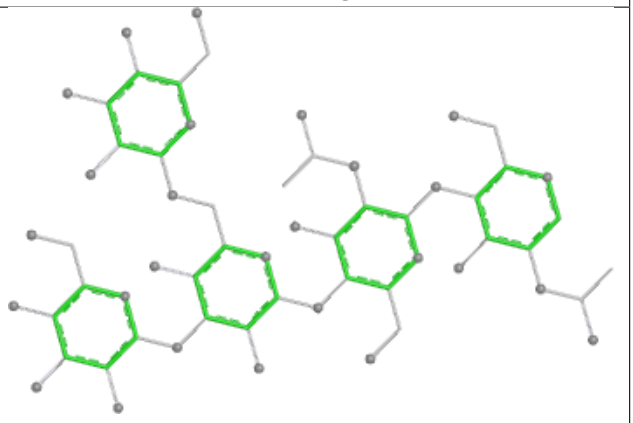
Bond lengths



Bond angles

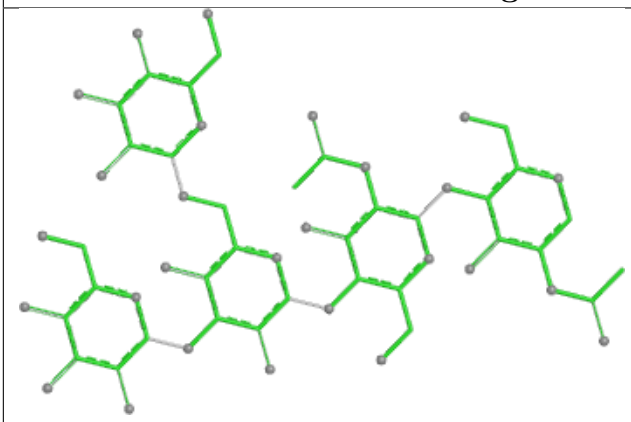


Torsions

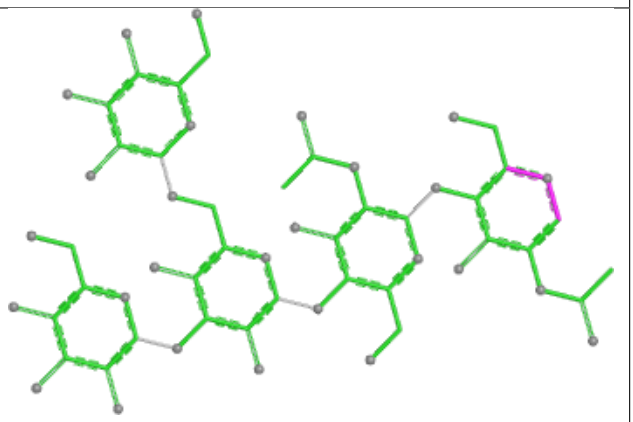


Rings

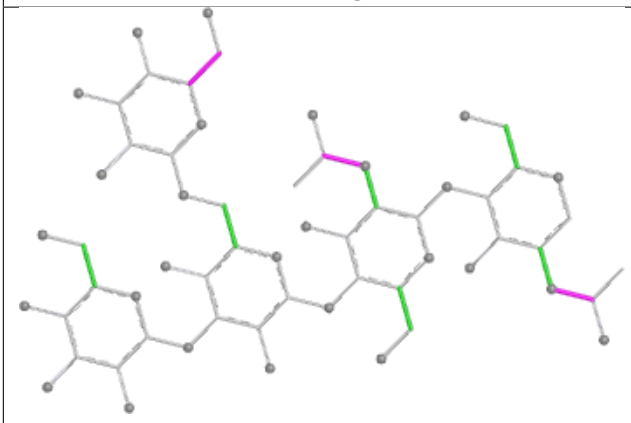
Oligosaccharide Chain I



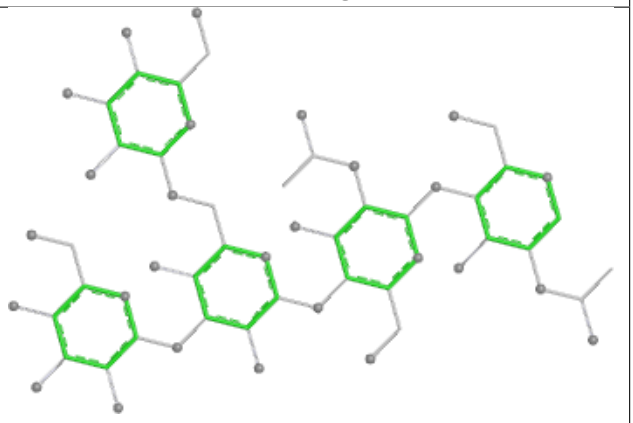
Bond lengths



Bond angles

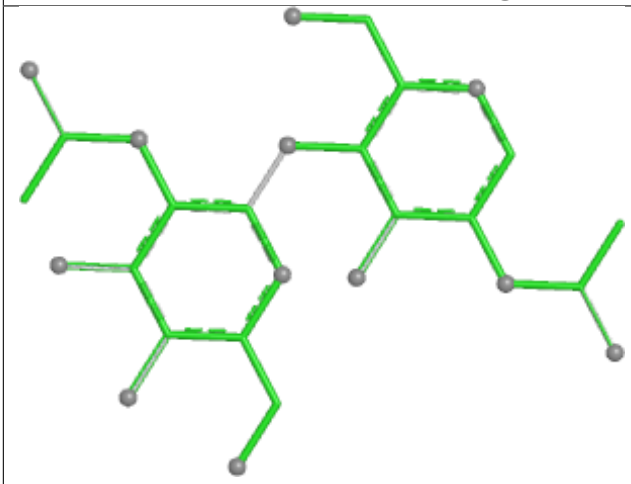


Torsions

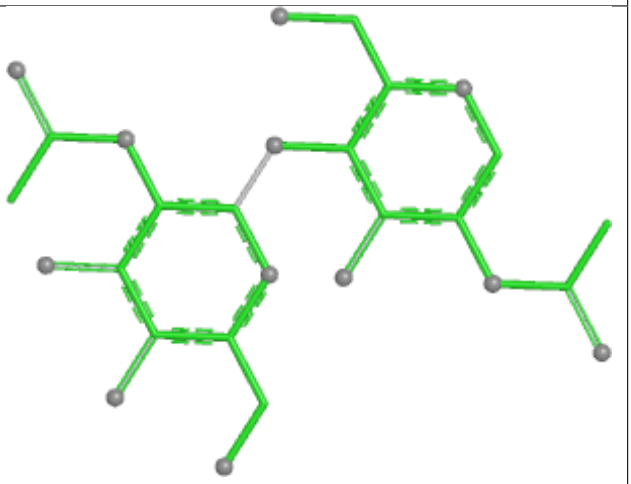


Rings

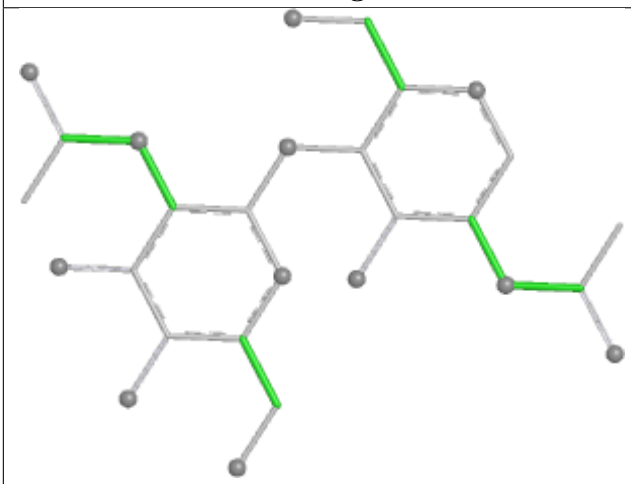
Oligosaccharide Chain F



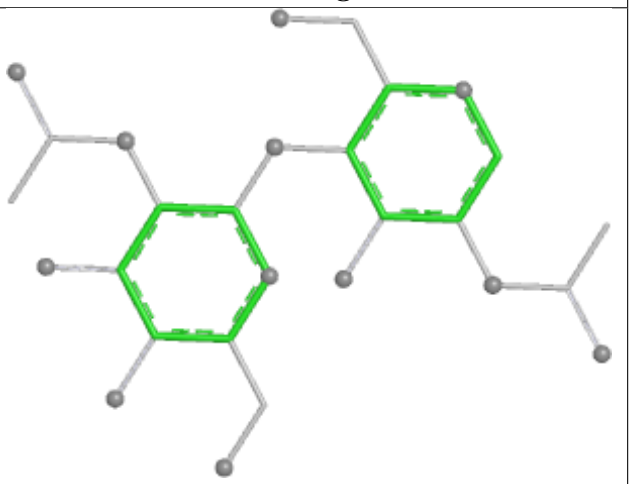
Bond lengths



Bond angles

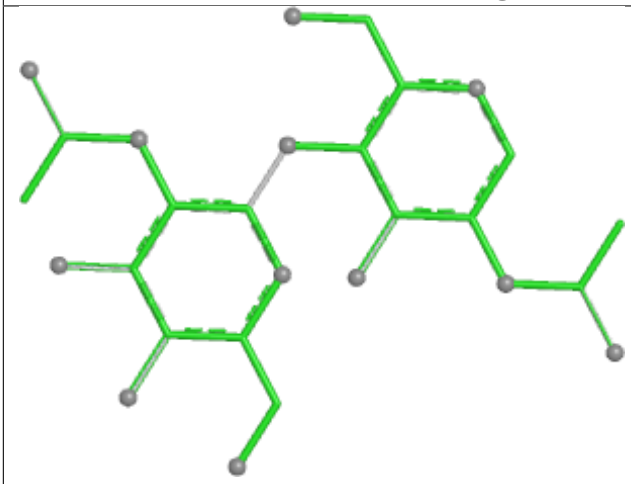


Torsions

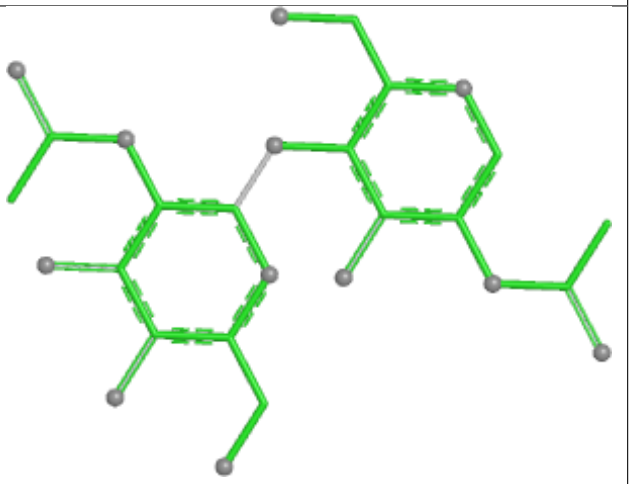


Rings

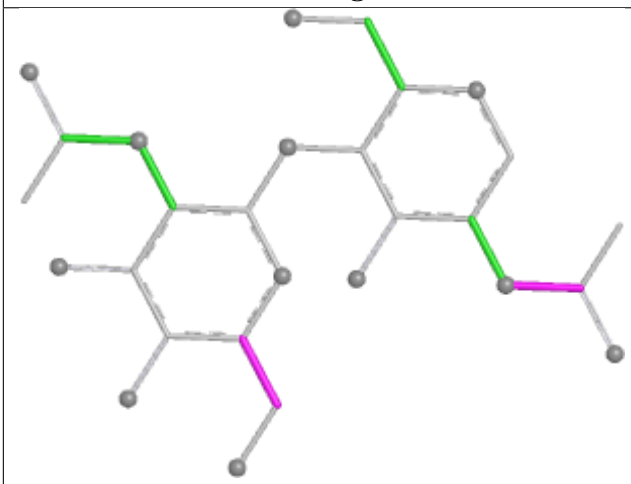
Oligosaccharide Chain G



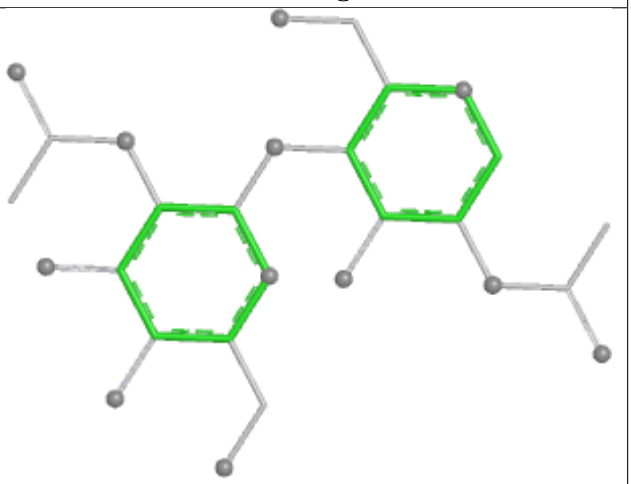
Bond lengths



Bond angles

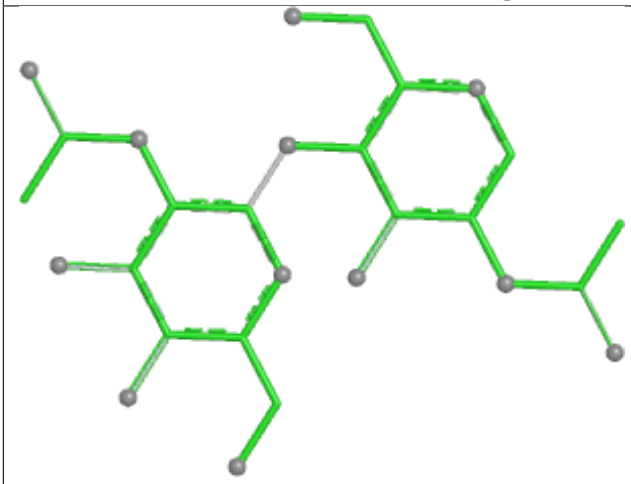


Torsions

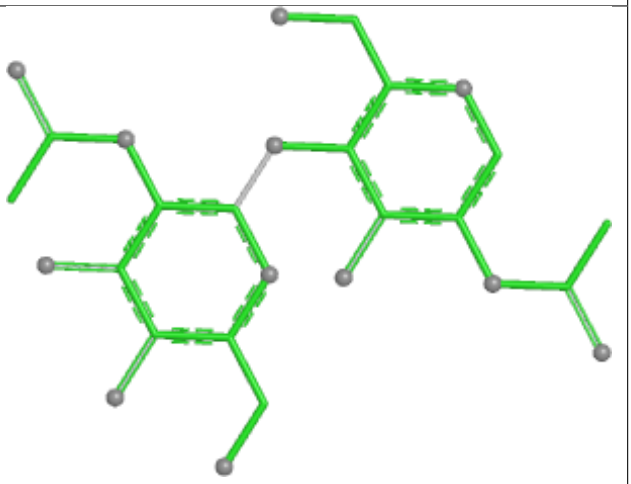


Rings

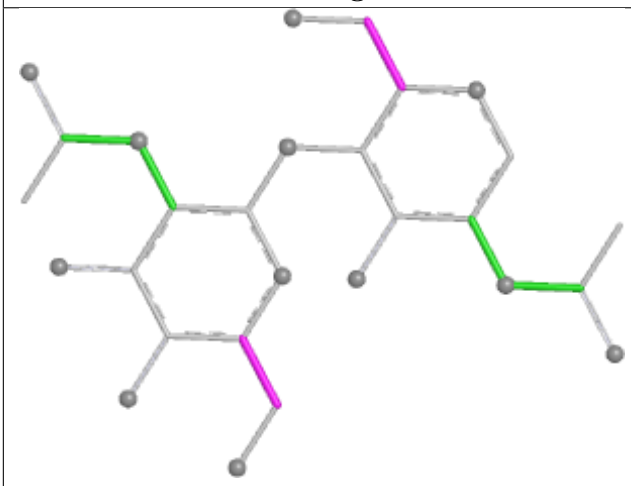
Oligosaccharide Chain J



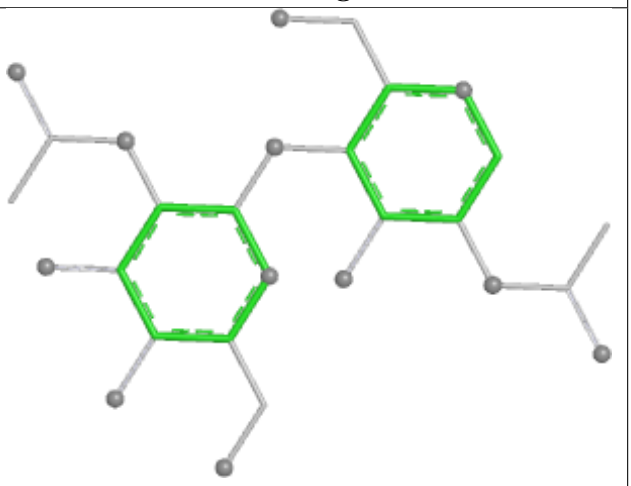
Bond lengths



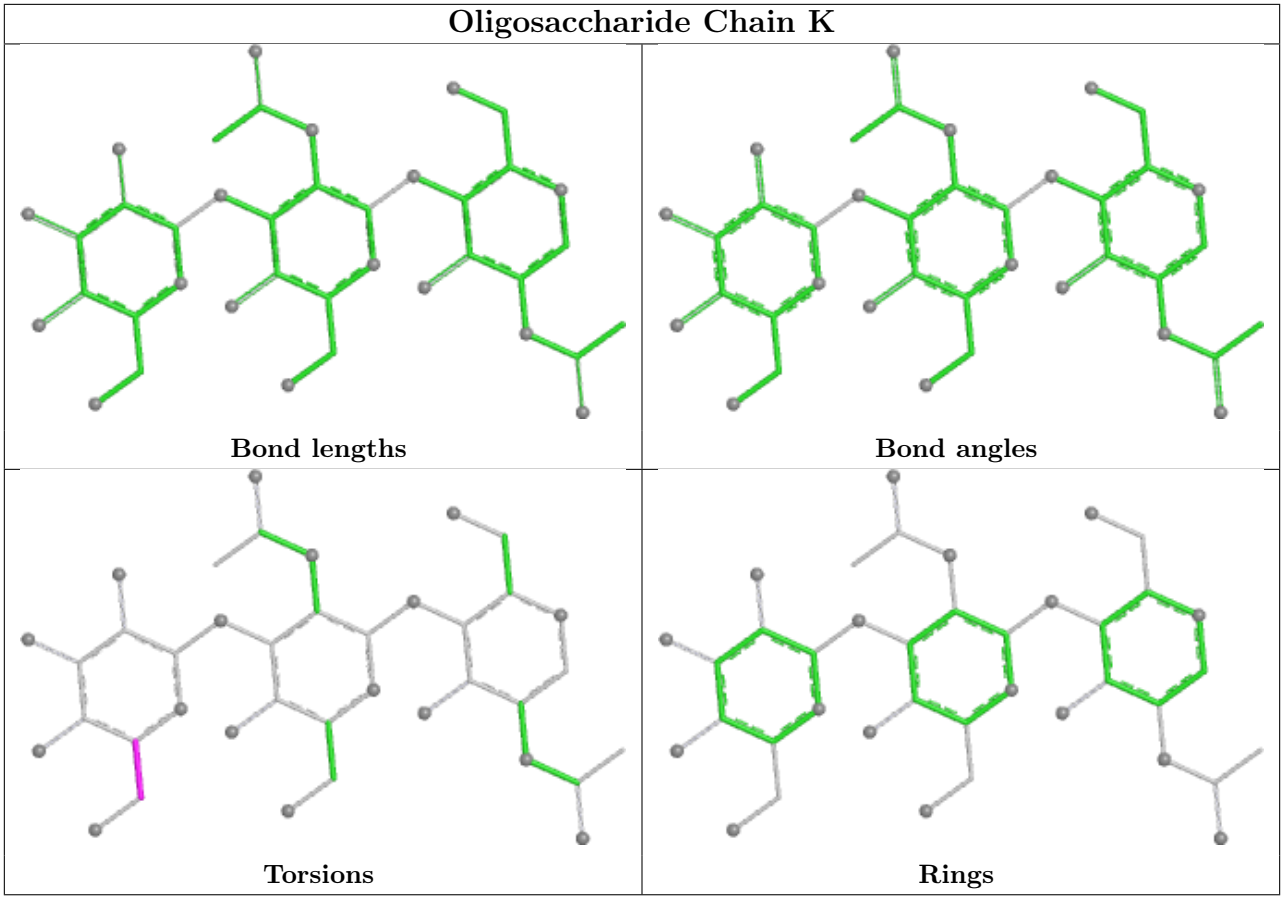
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
7	NAG	A	4701	1	14,14,15	0.31	0	17,19,21	0.57	0
7	NAG	A	4702	1	14,14,15	0.26	0	17,19,21	0.64	0
8	A2G	A	4703	1	14,14,15	0.40	0	17,19,21	0.72	0
8	A2G	A	4706	1	14,14,15	0.39	0	17,19,21	0.63	0
8	A2G	A	4707	1	14,14,15	0.39	0	17,19,21	0.61	0
8	A2G	A	4704	1	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
8	A2G	A	4705	1	14,14,15	0.42	0	17,19,21	0.55	0

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	4701	1	-	0/6/23/26	0/1/1/1
7	NAG	A	4702	1	-	3/6/23/26	0/1/1/1
8	A2G	A	4703	1	-	0/6/23/26	0/1/1/1
8	A2G	A	4706	1	-	0/6/23/26	0/1/1/1
8	A2G	A	4707	1	-	1/6/23/26	0/1/1/1
8	A2G	A	4704	1	-	0/6/23/26	0/1/1/1
8	A2G	A	4705	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	4704	A2G	C1-C2-N2	2.03	113.63	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4702	NAG	C1-C2-N2-C7
7	A	4702	NAG	C8-C7-N2-C2
7	A	4702	NAG	O7-C7-N2-C2
8	A	4707	A2G	O5-C5-C6-O6
8	A	4705	A2G	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

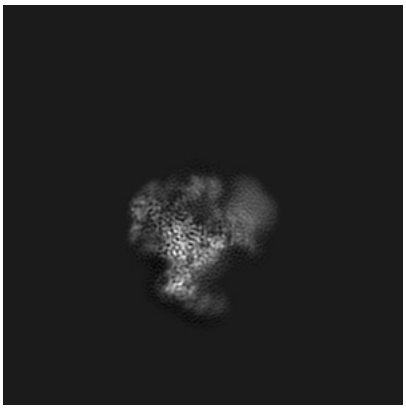
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36694. These allow visual inspection of the internal detail of the map and identification of artifacts.

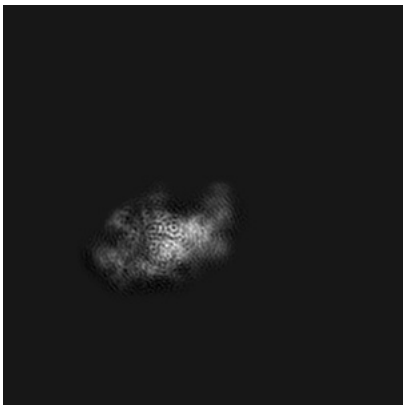
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

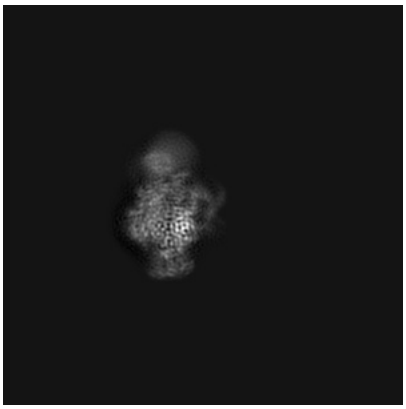
6.1.1 Primary map



X

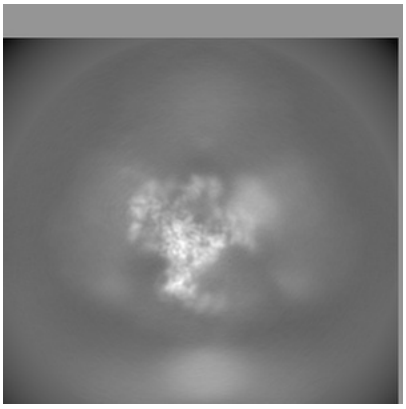


Y

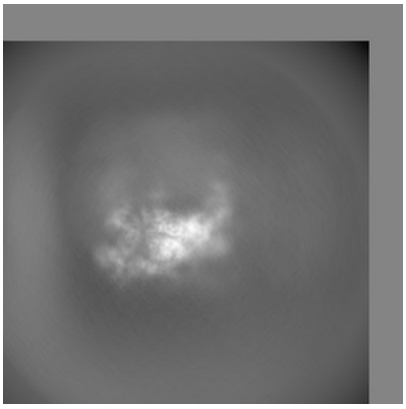


Z

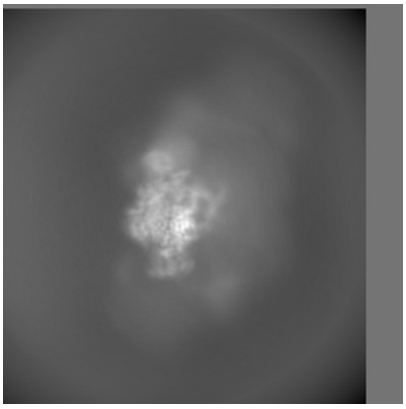
6.1.2 Raw map



X



Y

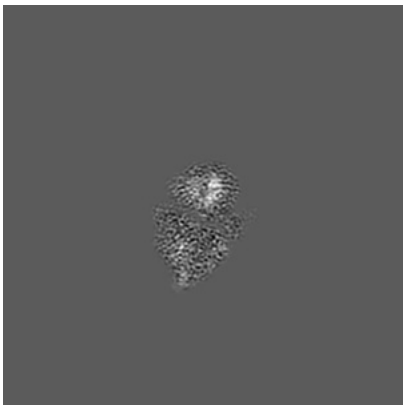


Z

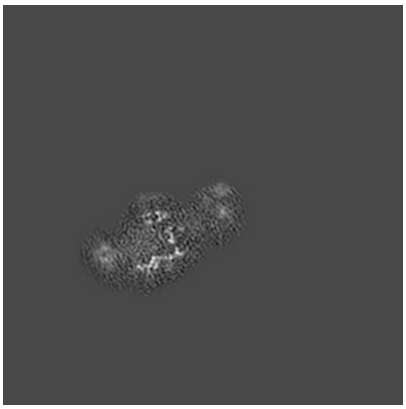
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

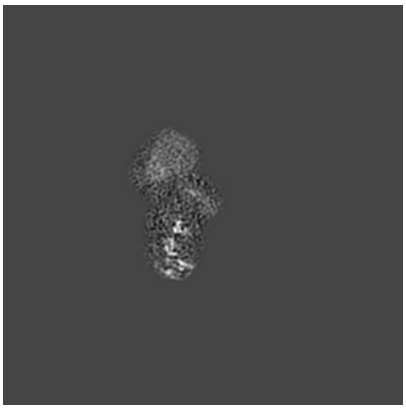
6.2.1 Primary map



X Index: 130

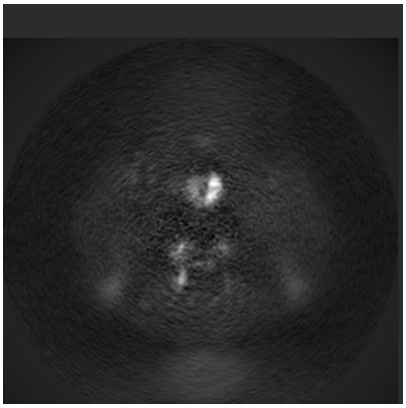


Y Index: 130

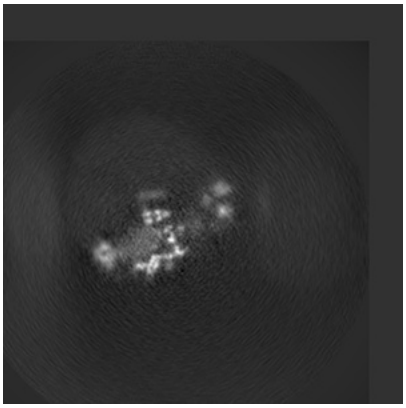


Z Index: 130

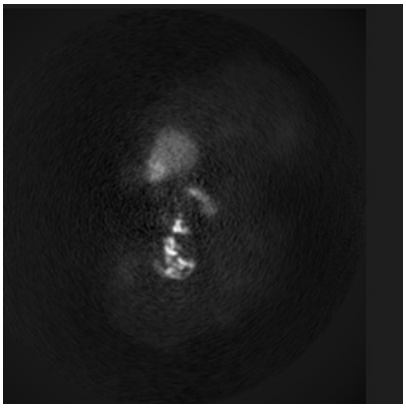
6.2.2 Raw map



X Index: 130



Y Index: 130

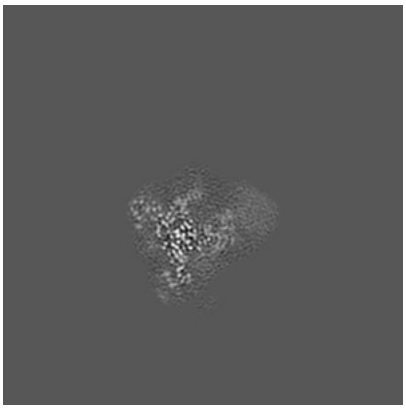


Z Index: 130

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

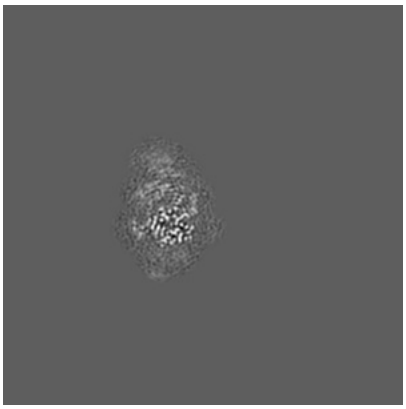
6.3 Largest variance slices (i)

6.3.1 Primary map



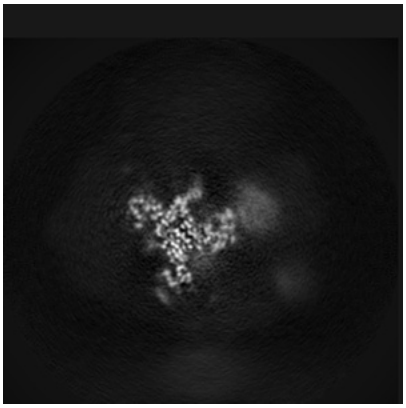
X Index: 113

Y Index: 115

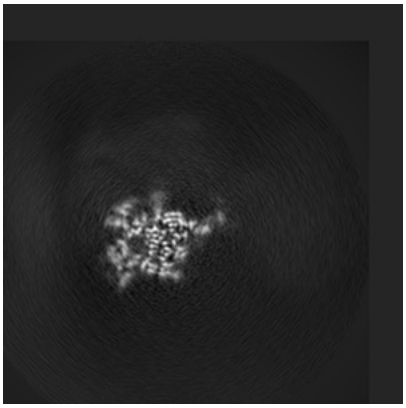


Z Index: 106

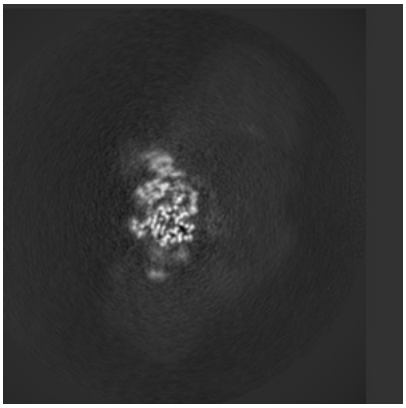
6.3.2 Raw map



X Index: 113



Y Index: 115

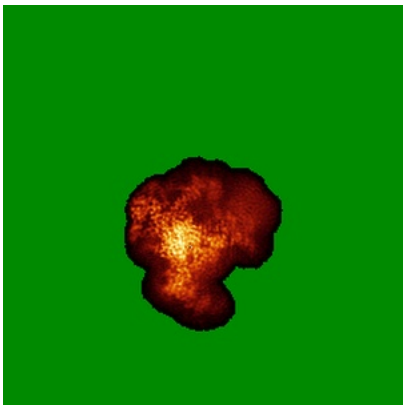


Z Index: 106

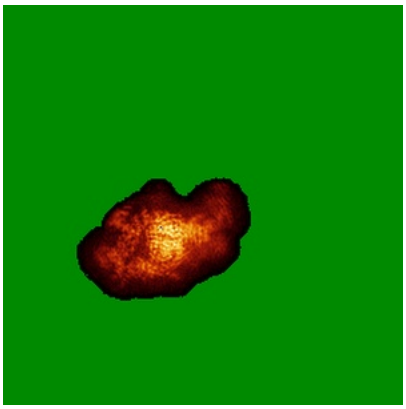
The images above show the largest variance slices of the map in three orthogonal directions.

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

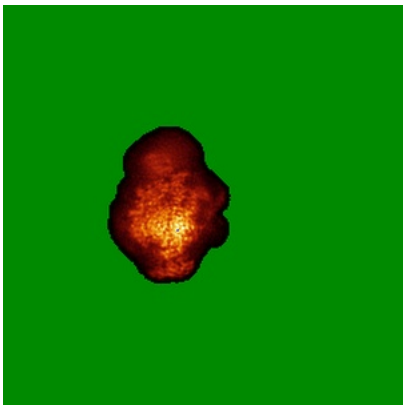
6.4.1 Primary map



X

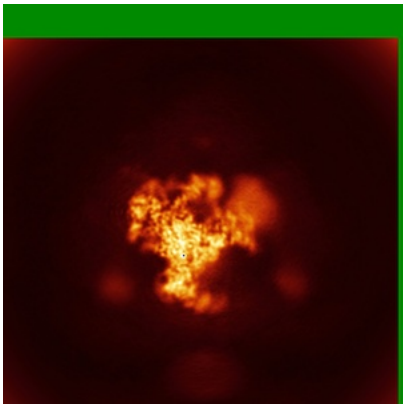


Y

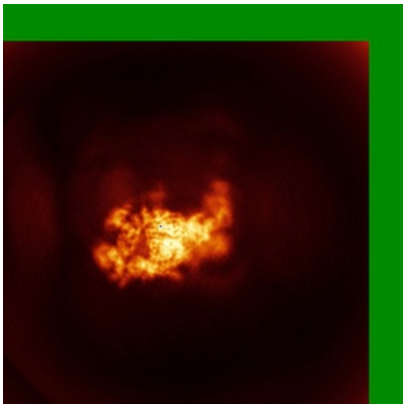


Z

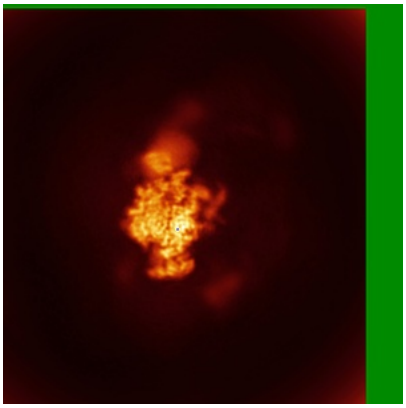
6.4.2 Raw map



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.

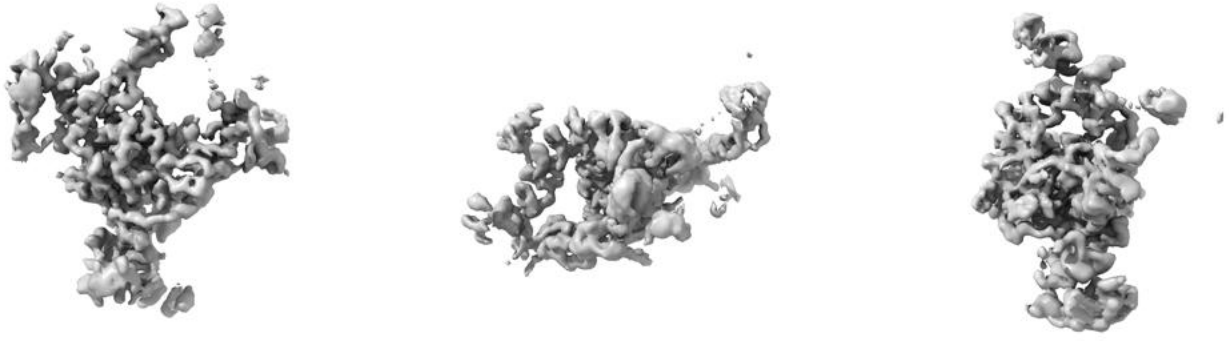
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0434. 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.

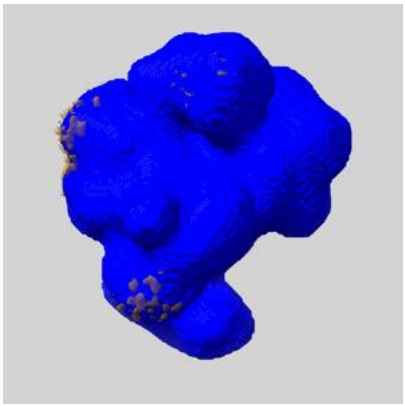
6.6 Mask visualisation (i)

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

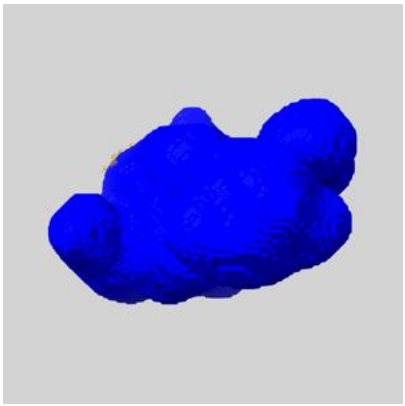
A mask typically either:

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

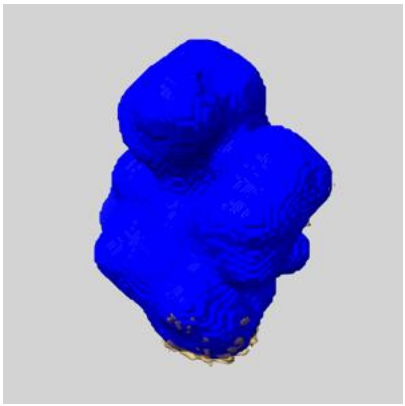
6.6.1 emd_36694_msk_1.map (i)



X



Y

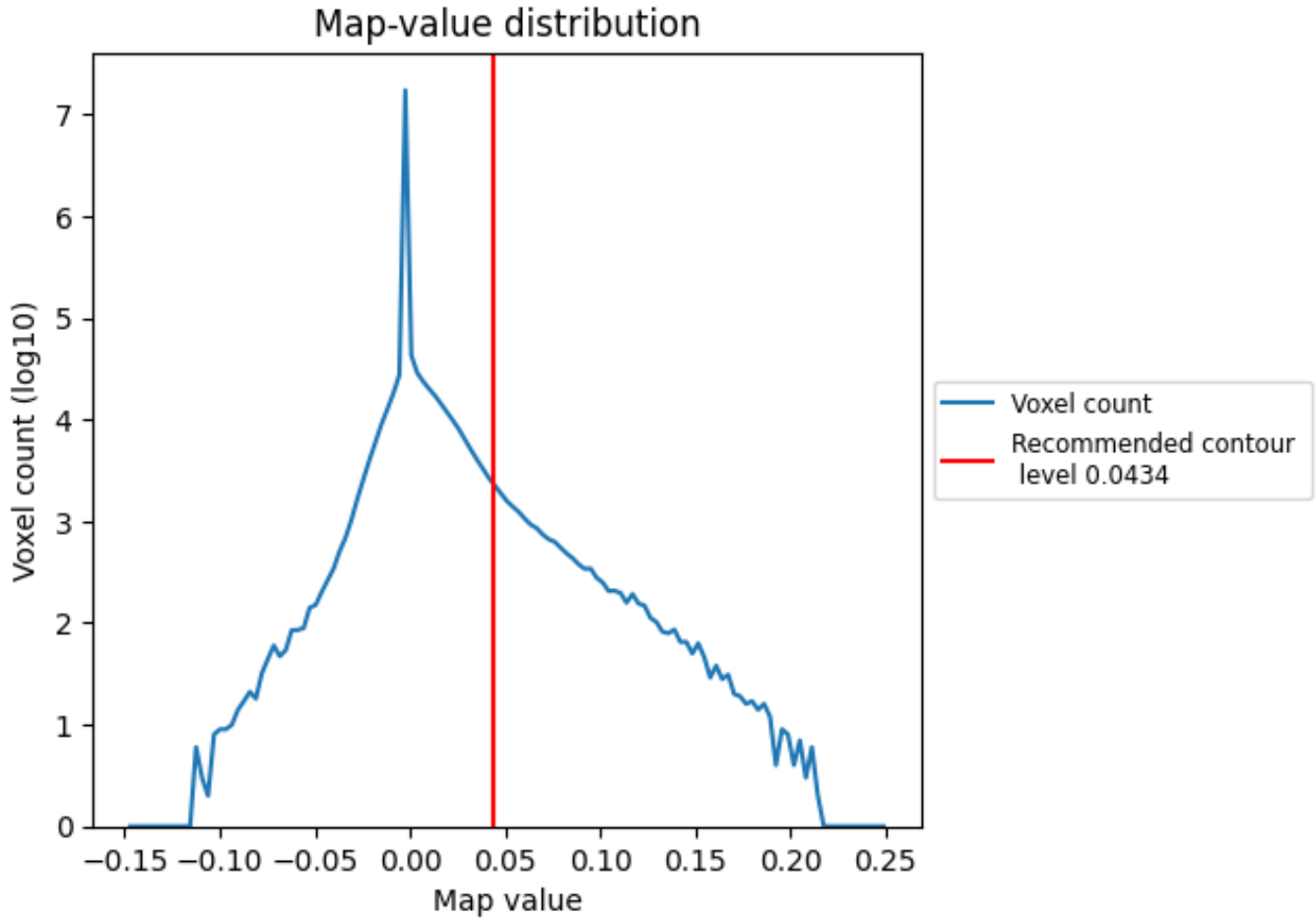


Z

7 Map analysis

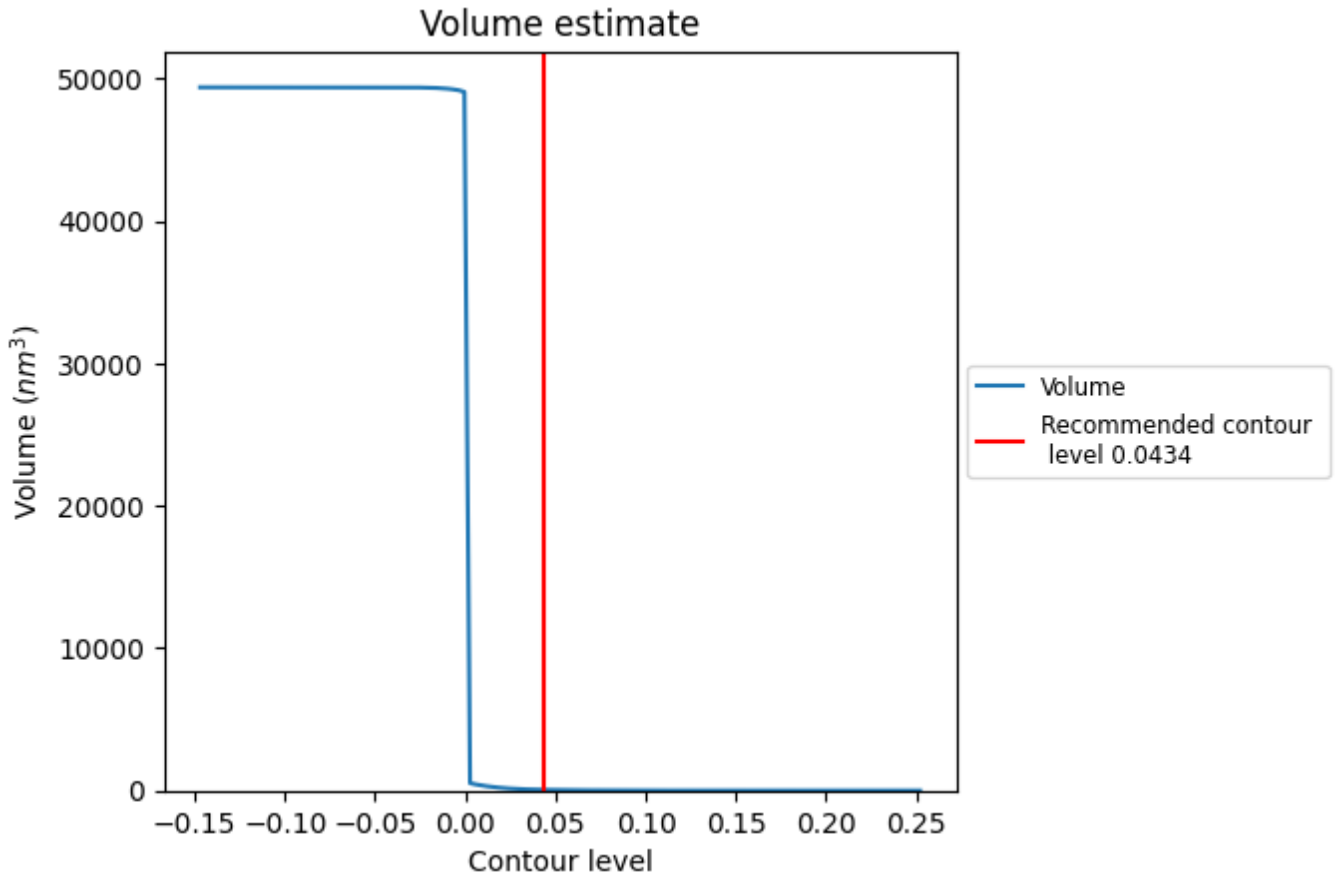
This section contains the results of statistical analysis of the map.

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.

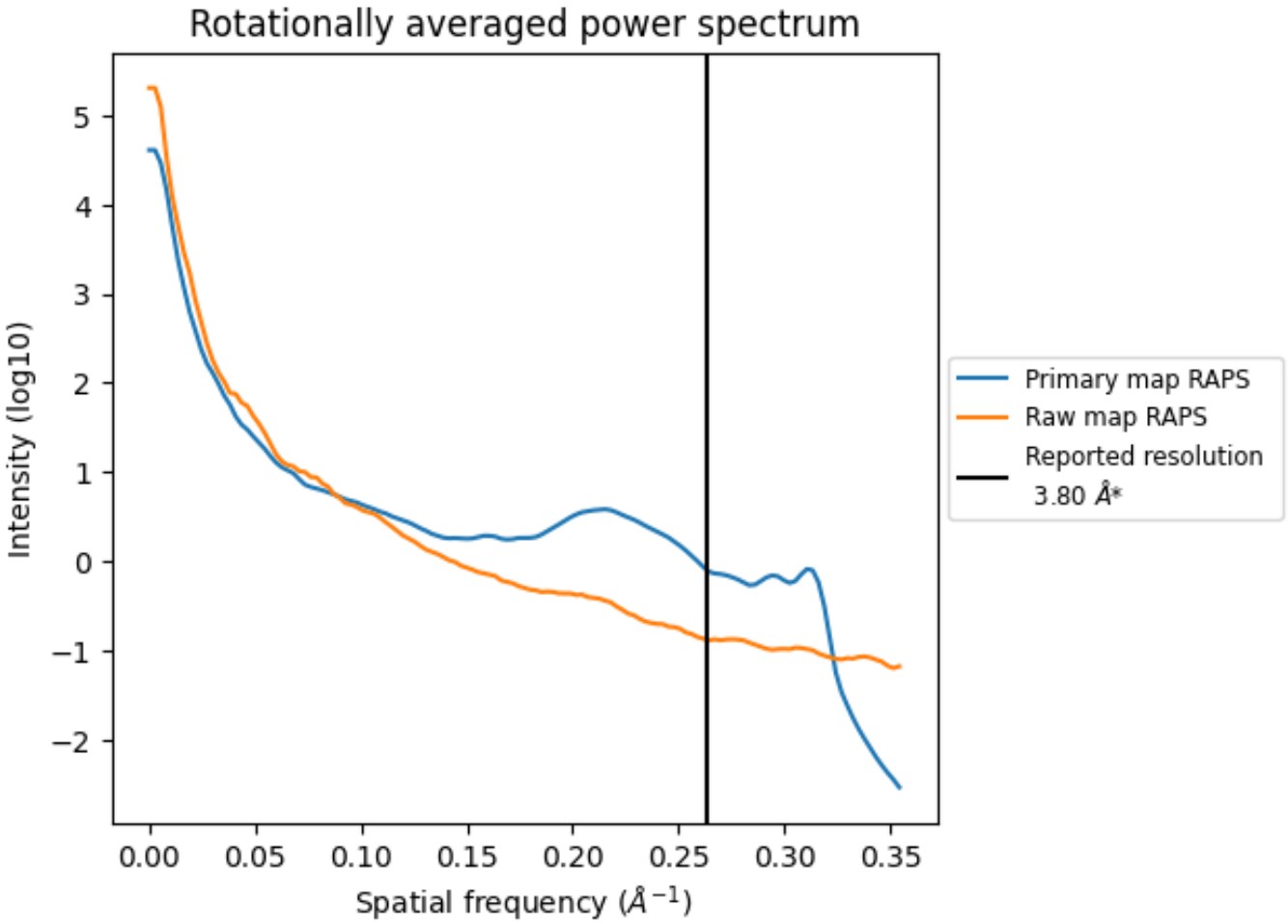
7.2 Volume estimate (i)



The volume at the recommended contour level is 55 nm^3; this corresponds to an approximate mass of 49 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)

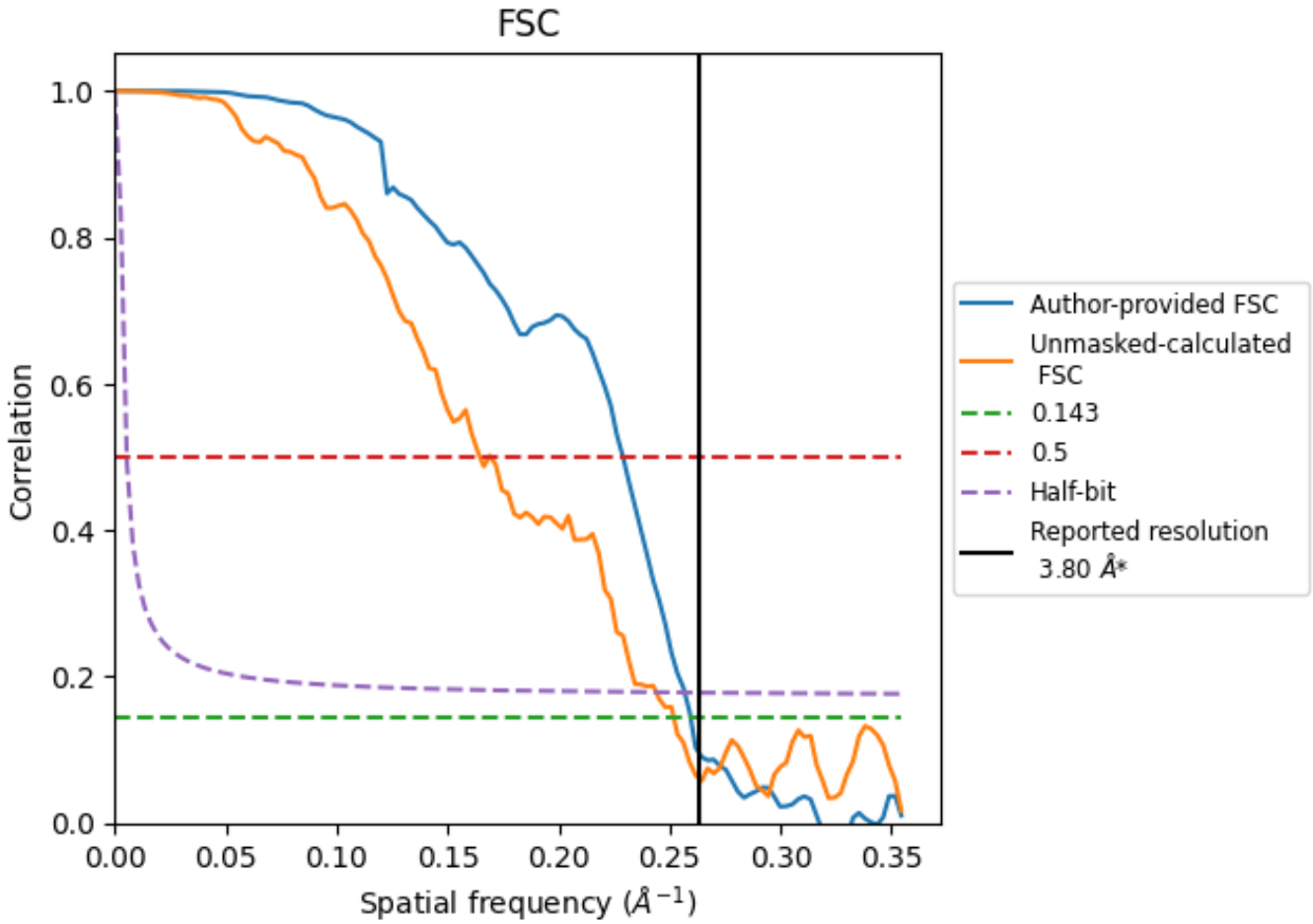


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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)

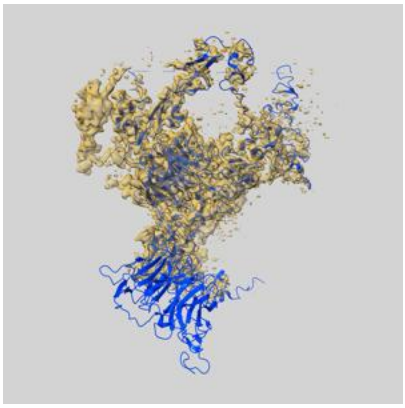
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.86	4.37	3.89
Unmasked-calculated*	3.97	6.08	4.10

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

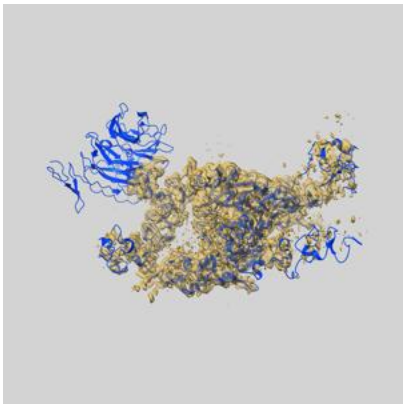
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36694 and PDB model 8JXA. Per-residue inclusion information can be found in section 3 on page 8.

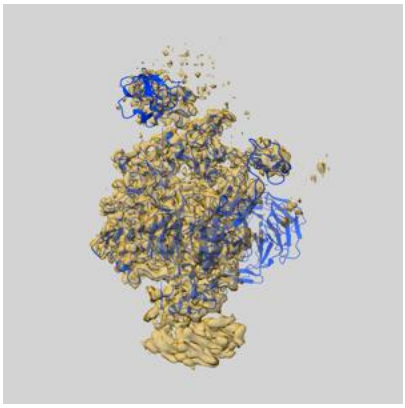
9.1 Map-model overlay



X



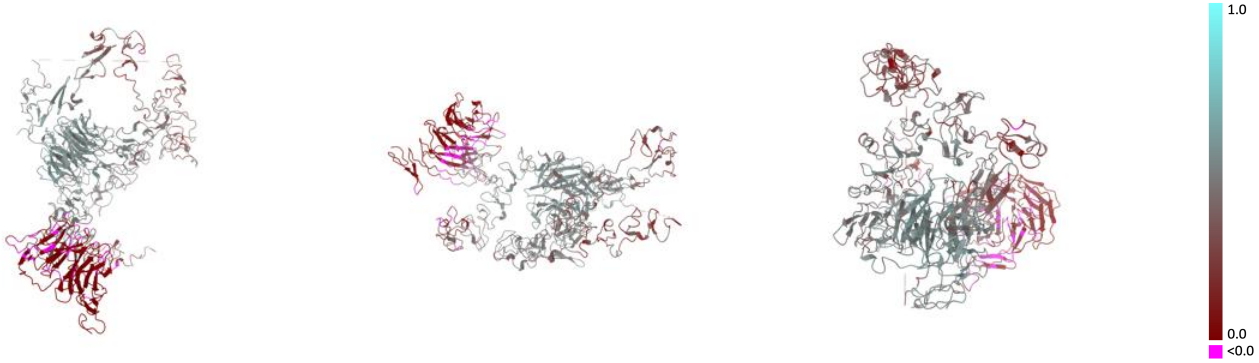
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0434 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.

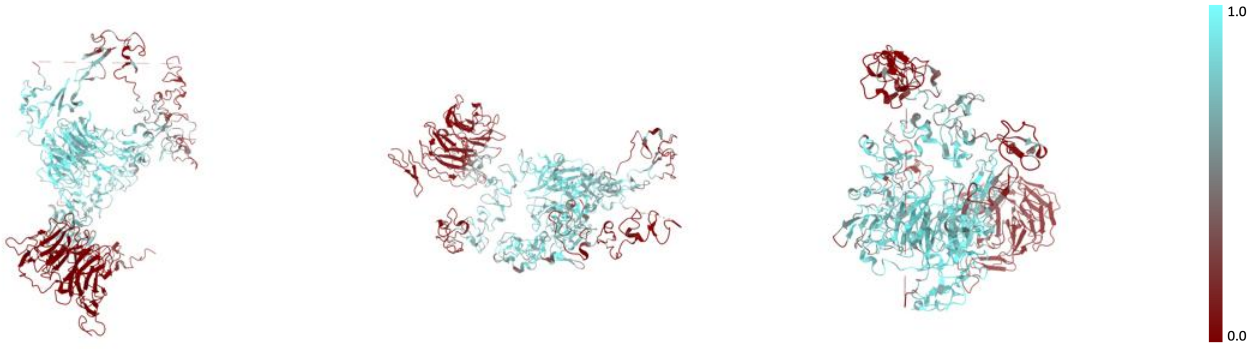
9.2 Q-score mapped to coordinate model



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.

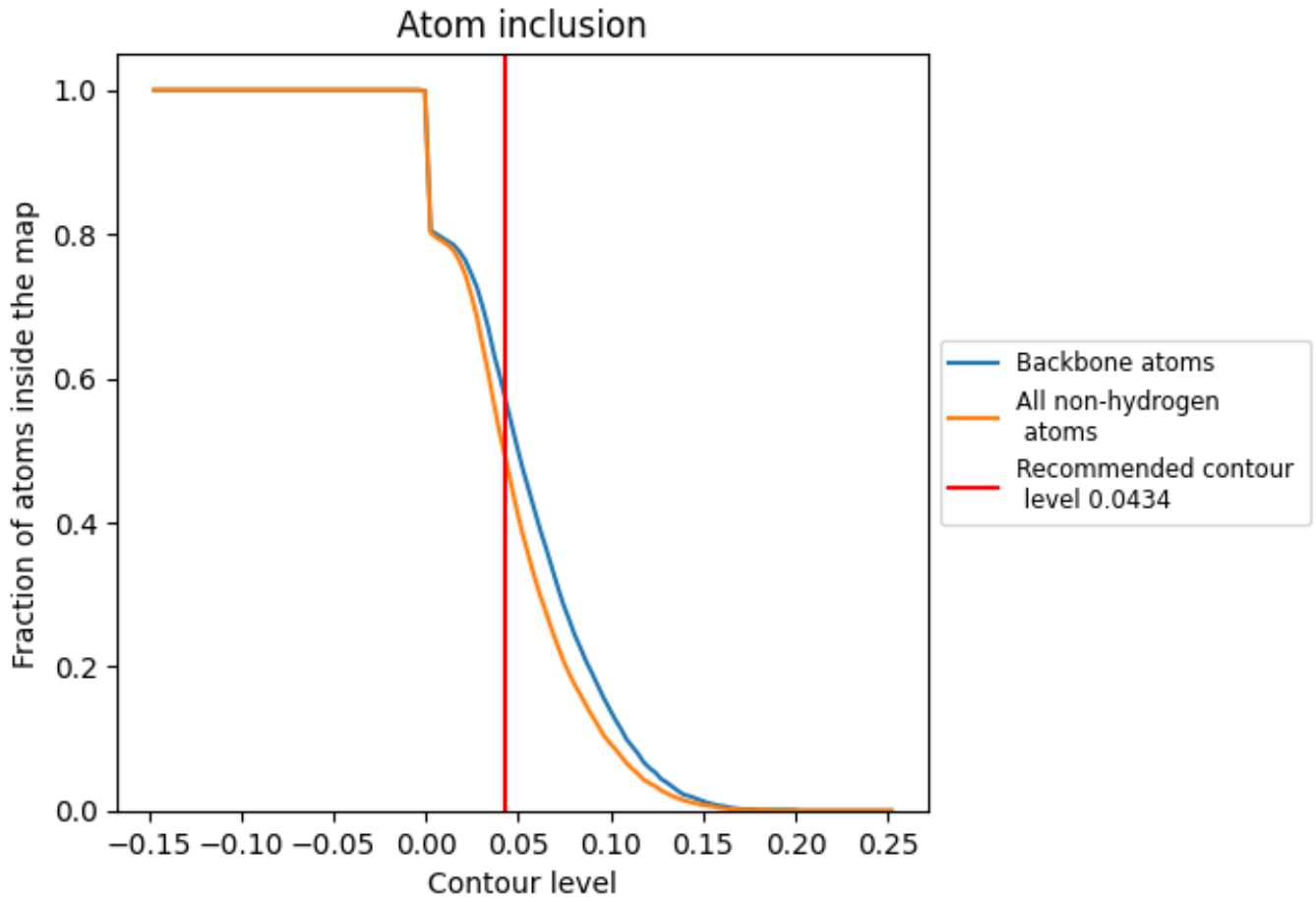
9.3 Atom inclusion mapped to coordinate model



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 (0.0434).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 48% 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 (0.0434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.3510
A	0.6310	0.4470
B	0.0620	0.0640
C	0.2560	0.3670
D	0.6150	0.4640
E	0.5250	0.4390
F	0.3210	0.4710
G	0.6430	0.5270
H	0.3930	0.3770
I	0.5570	0.4580
J	0.0000	0.0000
K	0.0000	0.0000
M	0.8930	0.5560