Full wwPDB EM Validation Report

Jun 12, 2024 – 10:14 AM JST

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

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

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

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

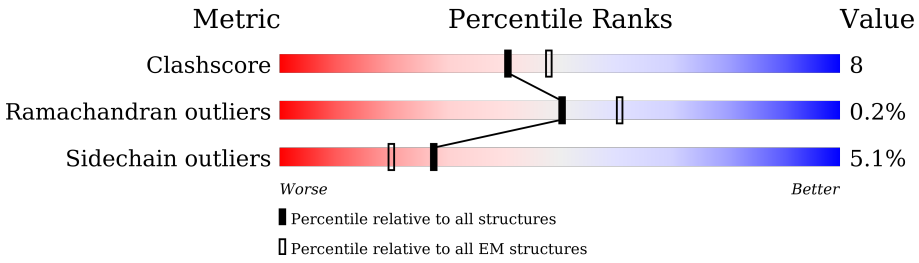
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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% 33% 33%
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	50% 100%
5	G	2	100%
5	J	2	100% 100%
6	K	3	100% 100%

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.

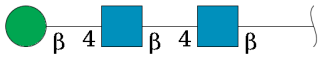
- Molecule 1 is a protein called LDL receptor related protein 2.

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.

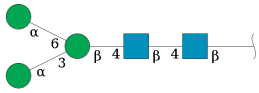
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	5	Total	C	N	O	0	0
			28	16	6	6		

- 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.

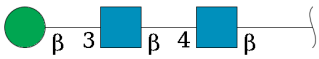


Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total 61	C 34	N 2	O 25	0	0
4	H	5	Total 61	C 34	N 2	O 25	0	0
4	I	5	Total 61	C 34	N 2	O 25	0	0

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

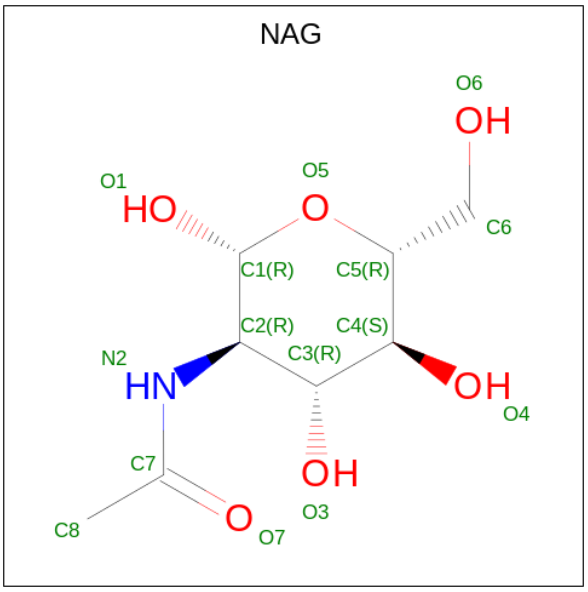
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	2	Total 28	C 16	N 2	O 10	0	0
5	G	2	Total 28	C 16	N 2	O 10	0	0
5	J	2	Total 28	C 16	N 2	O 10	0	0

- 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.



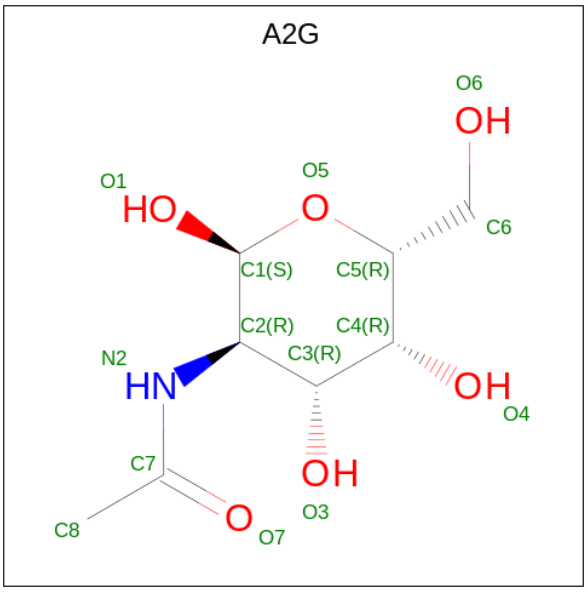
Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	3	Total 39	C 22	N 2	O 15	0	0

- 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).

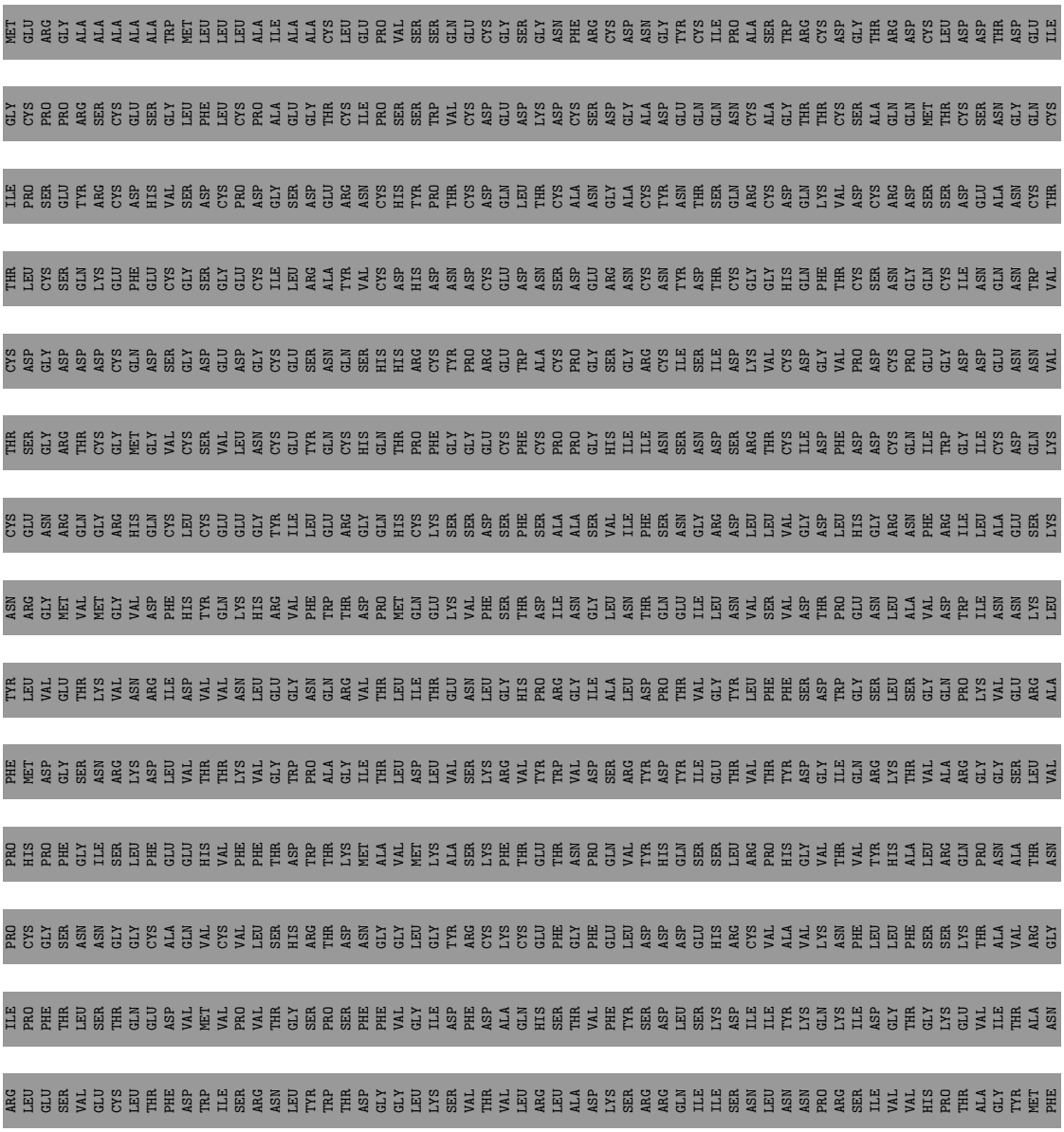
Mol	Chain	Residues	Atoms		AltConf
9	A	20	Total	Ca	0
			20	20	

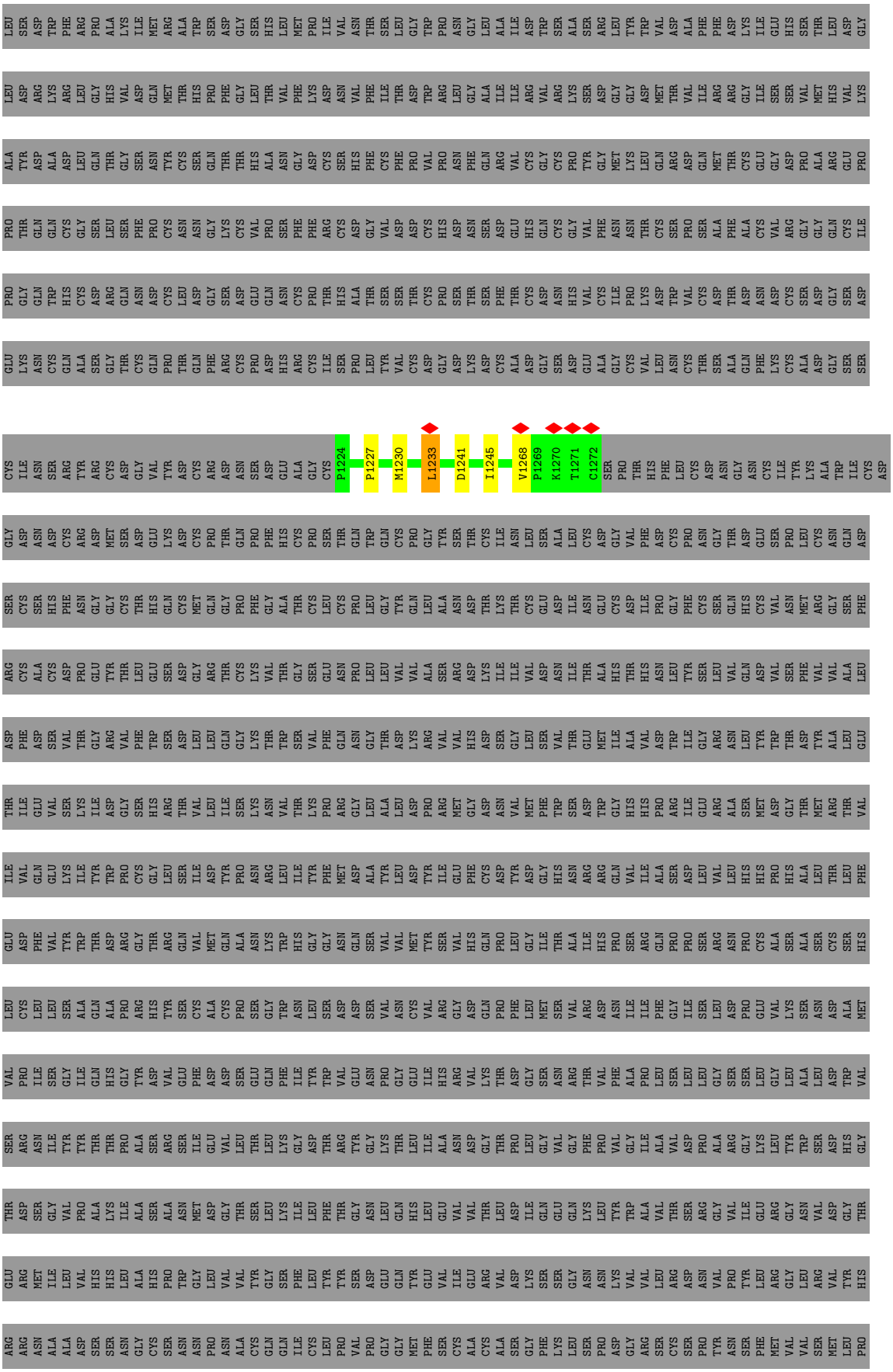
3 Residue-property plots (i)

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:

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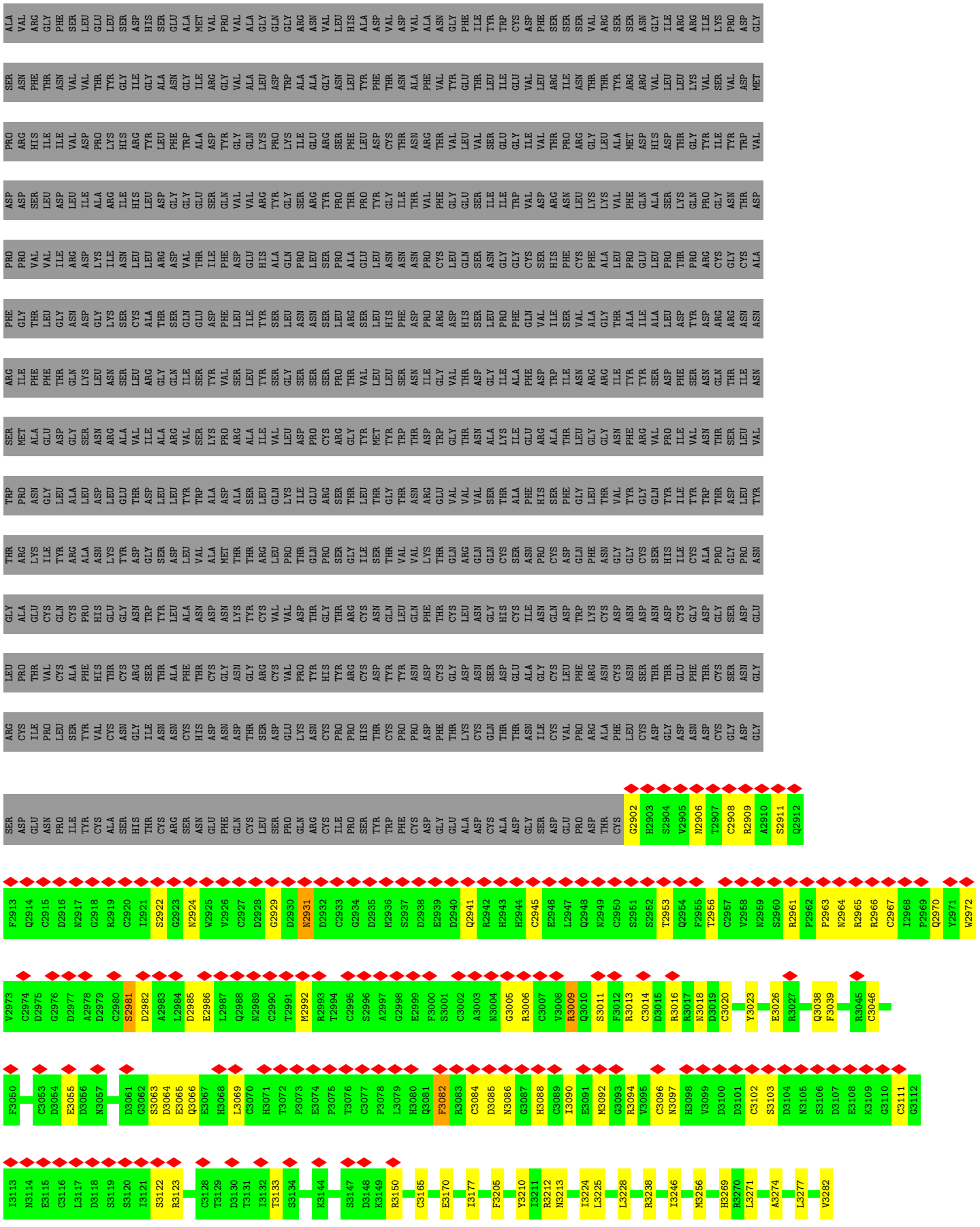
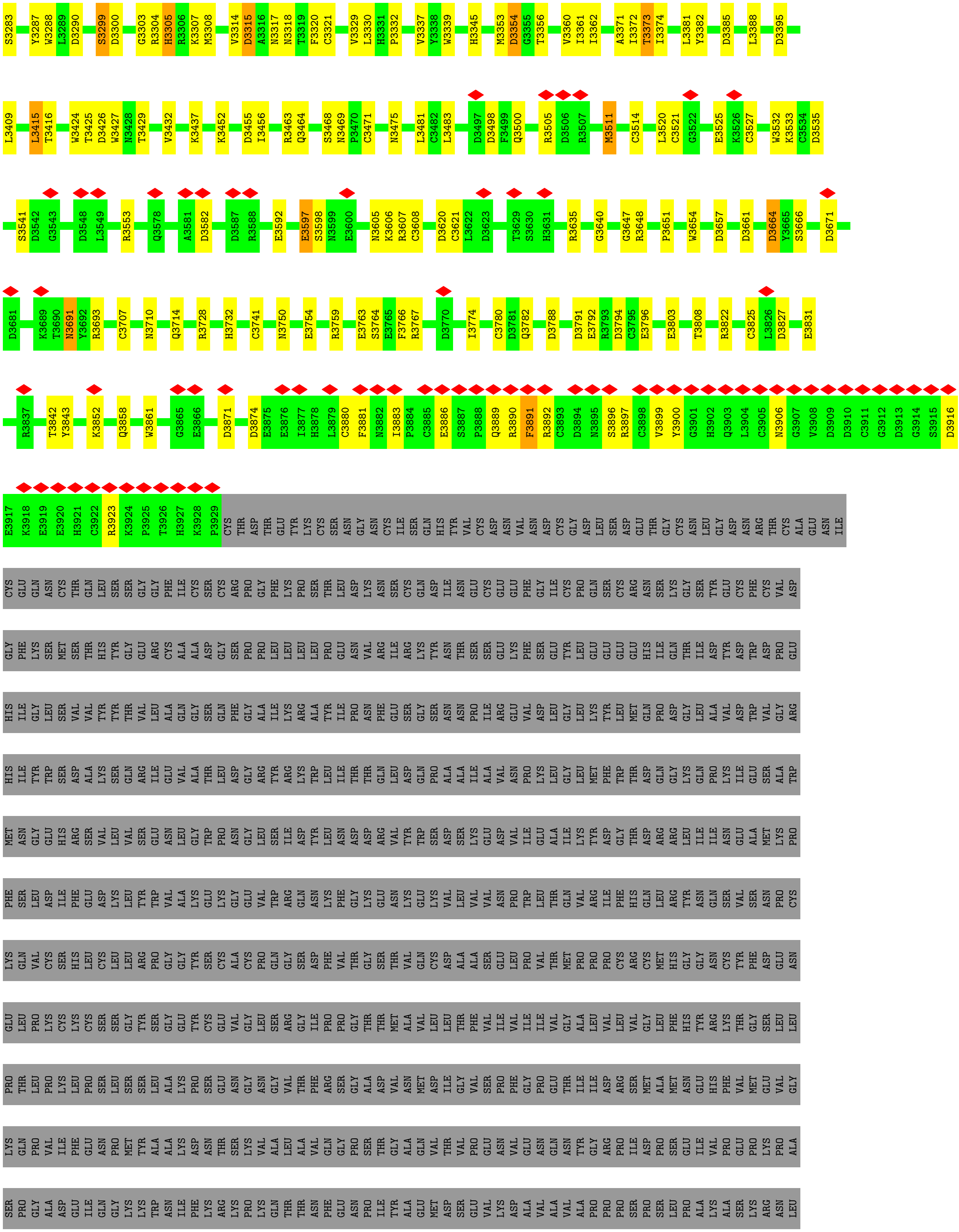
L1233
D1241
I1245
V1268
P1269
K1270
T1271
C1272

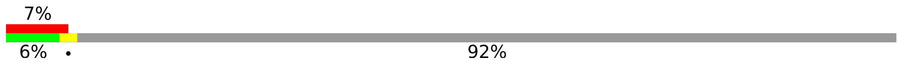



S3283 Y3287 W3288 L3289 D3290 S3299 D3300 G3303 R3304 H3305 R3306 K3307 M3308 V3314 D3315 A3316 N3317 N3318 T3319 F3320 C3321 V3329 L3330 H3331 P3332 V3337 Y3338 W3339 H3345 M3353 D3354 G3355 T3356 V3360 I3361 I3362 A3371 I3372 T3373 I3374 L3381 Y3382 D3385 L3388 D3395
L3409 L3415 T3416 W3424 T3425 D3426 W3427 N3428 T3429 V3432 K3437 K3452 D3455 I3456 R3463 Q3464 S3468 N3469 P3470 C3471 N3475 L3481 C3482 L3483 D3497 D3498 F3499 Q3500 R3505 D3506 R3507 M3511 C3514 L3520 C3521 G3522 E3525 K3526 C3527 W3532 K3533 C3534 D3535
S3541 D3542 G3543 D3548 L3549 R3553 Q3578 A3581 D3582 D3587 R3588 E3592 E3597 S3598 N3599 E3600 N3605 K3606 R3607 C3608 D3620 C3621 L3622 D3623 T3629 S3630 H3631 R3635 G3640 G3647 R3648 P3651 W3654 D3657 D3661 D3664 Y3665 S3666 D3671
D3681 K3689 T3690 N3691 Y3692 R3693 C3707 N3710 Q3714 R3728 H3732 C3741 N3750 E3754 R3759 E3763 S3764 E3765 F3766 R3767 D3770 I3774 C3780 D3781 Q3782 D3788 D3791 E3792 R3793 D3794 C3795 E3796 E3803 T3808 R3822 C3825 L3826 D3827 E3831
R3837 T3842 Y3843 K3852 Q3858 W3861 G3865 E3866 D3871 D3874 E3875 E3876 I3877 H3878 L3879 C3880 F3881 N3882 I3883 P3884 C3885 E3886 S3887 P3888 Q3889 R3890 F3891 R3892 C3893 D3894 N3895 S3896 R3897 C3898 V3899 Y3900 G3901 H3902 Q3903 L3904 C3905 N3906 G3907 V3908 D3909 D3910 C3911 G3912 D3913 G3914 S3915 D3916
E3917 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 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 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 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 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 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

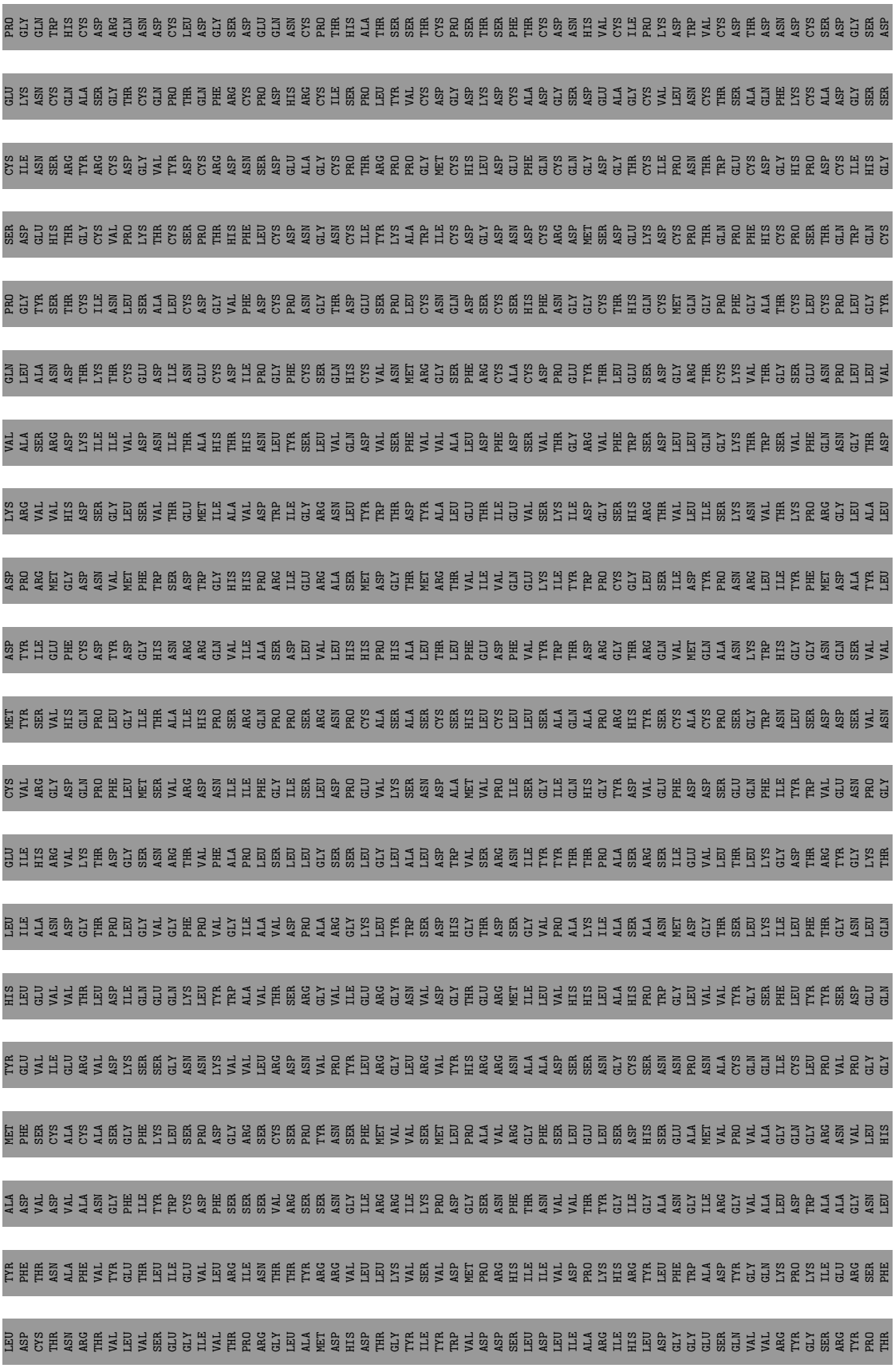
ARG LEU GLU SER VAL GLU CYS LEU THR PHE ASP TRP ILE SER ARG ASN LEU TYR TRP THR ASP GLY GLY LEU LYS SER VAL THR VAL LEU ARG LEU ALA ASP LYS SER ARG ARG GLN ILE ILE SER ASN LEU ASN ASN PRO ARG SER ILE VAL VAL HIS PRO THR ALA GLY TYR MET PHE

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 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

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

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 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

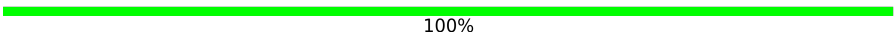
ALA MET ASN GLU HIS PHE VAL MET GLU VAL GLY LYS GLN PRO VAL ILE PHE GLU ASN PRO MET TYR ALA ALA LYS ASP ASN THR SER LYS VAL ALA LEU ALA VAL GLN GLY PRO SER THR GLY ALA GLN VAL THR VAL PRO GLU ASN VAL GLU ASN GLN ASN TYR GLY ARG PRO ILE ASP

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:



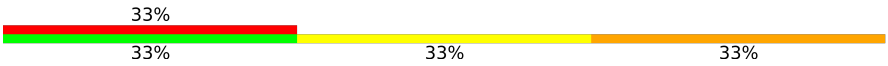
There are no outlier residues recorded for this chain.

• 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:

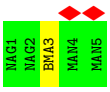
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



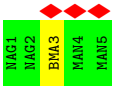
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



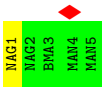
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



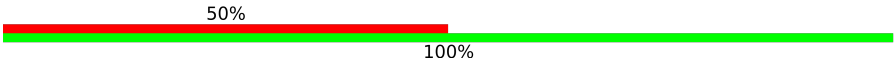
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: MAN, BMA, CA, A2G, 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.

All (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
1:A:2961:ARG:HG2	1:A:2963:PRO:HD2	1.78	0.66
1:A:3525:GLU:OE2	1:A:3525:GLU:N	2.26	0.65
1:A:3329:VAL:HG11	1:A:3373:THR:HA	1.77	0.65
1:A:3282:VAL:O	1:A:3469:ASN:ND2	2.30	0.64
1:B:4141:LYS:O	1:B:4178:ARG:NH2	2.20	0.64
1:A:3085:ASP:OD2	1:A:3086:ASN:ND2	2.30	0.64
1:A:3305:HIS:HB3	1:A:3481:LEU:CD2	2.31	0.61
1:A:2929:GLY:HA2	1:A:2966:ARG:HB3	1.83	0.61
1:A:3880:CYS:HA	1:A:3883:ILE:HB	1.82	0.60
1:B:4168:ILE:HG23	1:B:4181:LEU:HB2	1.84	0.60
1:B:4180:TRP:N	1:B:4357:GLN:OE1	2.33	0.60
1:A:3597:GLU:HG3	1:A:3598:SER:H	1.66	0.60
1:B:4375:LEU:HD23	1:B:4375:LEU:H	1.66	0.59
1:A:1233:LEU:HD23	1:A:1233:LEU:H	1.67	0.59
1:B:4061:PRO:HG3	1:B:4089:ILE:HG12	1.84	0.59
1:A:3455:ASP:OD1	1:A:3456:ILE:N	2.36	0.58
1:A:3094:ARG:HD3	1:A:3097:ASN:HD21	1.68	0.57
1:A:3385:ASP:OD1	1:A:3388:LEU:N	2.36	0.57
1:A:3607:ARG:NH2	1:A:3620:ASP:O	2.37	0.57
1:A:3314:VAL:O	1:A:3315:ASP:HB3	2.05	0.57
1:A:3759:ARG:O	1:A:3767:ARG:NH2	2.32	0.56
1:A:3782:GLN:HE22	1:A:3825:CYS:HA	1.70	0.56
1:A:3794:ASP:OD2	1:B:4167:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2981:SER:OG	1:A:2982:ASP:N	2.39	0.56
1:A:3886:GLU:OE1	1:A:3889:GLN:NE2	2.34	0.55
1:B:4138:LEU:HD22	1:B:4174:ASP:HA	1.88	0.55
1:A:3766:PHE:HD2	1:A:3774:ILE:HD11	1.70	0.55
1:B:4106:THR:HG21	1:B:4146:PRO:HB2	1.89	0.55
1:B:4213:GLU:HG2	1:B:4224:VAL:HG22	1.88	0.55
1:A:3122:SER:O	1:A:3150:ARG:NH1	2.40	0.55
1:A:3657:ASP:OD1	1:A:3693:ARG:NH2	2.33	0.55
1:A:3664:ASP:OD2	1:A:3664:ASP:N	2.38	0.55
1:B:4163:ALA:HA	1:B:4189:PRO:HG2	1.87	0.55
1:B:4176:ARG:HG3	1:B:4176:ARG:HH11	1.72	0.55
1:A:2956:THR:O	1:A:2965:ARG:NH1	2.40	0.54
1:A:3332:PRO:HA	1:A:3353:MET:HE3	1.89	0.54
1:A:3055:GLU:N	1:A:3065:GLU:OE1	2.40	0.54
1:A:2953:THR:O	1:A:2970:GLN:NE2	2.41	0.53
1:A:2985:ASP:OD1	1:A:2986:GLU:N	2.42	0.53
1:A:3288:TRP:HZ3	1:A:3299:SER:HB3	1.73	0.53
1:A:3354:ASP:OD1	1:A:3356:THR:HG22	2.09	0.53
1:A:3635:ARG:NH1	1:A:3647:GLY:O	2.42	0.52
1:A:3471:CYS:HB3	1:A:3475:ASN:HA	1.91	0.52
1:A:3005:GLY:HA3	1:A:3020:CYS:HB3	1.92	0.51
1:A:3304:ARG:O	1:A:3305:HIS:HB2	2.10	0.51
1:B:4093:TRP:CE2	1:B:4325:GLN:HB3	2.46	0.51
1:A:3082:PHE:CZ	1:A:3084:CYS:HB3	2.46	0.51
1:A:3329:VAL:HG13	1:A:3372:ILE:HG23	1.92	0.51
1:B:4162:ASP:HB3	1:B:4165:SER:HB2	1.92	0.51
1:A:3064:ASP:N	1:A:3064:ASP:OD1	2.44	0.51
1:A:2986:GLU:HG3	1:A:3006:ARG:HD2	1.93	0.50
1:A:3426:ASP:OD2	1:A:3429:THR:OG1	2.27	0.50
1:A:3592:GLU:O	1:A:3606:LYS:NZ	2.45	0.50
1:A:3283:SER:HA	1:A:3469:ASN:HD21	1.77	0.49
1:A:3520:LEU:HD13	1:A:3521:CYS:O	2.13	0.49
1:A:3300:ASP:OD1	1:A:3303:GLY:N	2.46	0.49
1:A:3287:TYR:OH	1:A:3353:MET:HB3	2.13	0.49
1:B:4087:GLN:HG2	1:B:4147:ASP:HA	1.94	0.49
1:A:3500:GLN:HB3	1:A:3511:MET:SD	2.53	0.49
1:A:2964:ASN:HD22	1:A:2981:SER:HB2	1.77	0.48
1:A:3063:SER:HA	1:A:3066:GLN:HG3	1.95	0.48
1:A:3520:LEU:HD23	1:A:3527:CYS:SG	2.53	0.48
1:B:4084:GLU:OE2	1:B:4110:GLN:NE2	2.47	0.48
1:A:3874:ASP:OD1	1:A:3874:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3651:PRO:HD2	1:A:3654:TRP:CE3	2.49	0.47
1:A:3803:GLU:OE2	1:A:3803:GLU:N	2.37	0.47
1:B:4163:ALA:HB1	1:B:4188:GLN:NE2	2.29	0.47
1:A:3210:TYR:OH	1:A:3764:SER:N	2.46	0.47
1:A:3791:ASP:OD1	1:A:3792:GLU:N	2.47	0.47
1:B:4193:ALA:HB3	1:B:4202:PHE:HB2	1.97	0.47
1:B:4180:TRP:CE2	1:B:4357:GLN:HG2	2.50	0.47
1:A:3916:ASP:OD1	1:A:3916:ASP:N	2.44	0.47
1:A:3330:LEU:HD22	1:A:3337:VAL:HG22	1.98	0.46
1:A:3371:ALA:HB1	1:A:3415:LEU:HD23	1.98	0.46
1:A:3096:CYS:SG	1:A:3133:THR:HG22	2.56	0.46
1:A:3822:ARG:N	1:A:3831:GLU:OE2	2.49	0.46
1:A:3205:PHE:HA	1:A:3456:ILE:HA	1.97	0.46
1:B:4091:TYR:HA	1:B:4103:VAL:HA	1.98	0.46
1:A:3858:GLN:HB2	1:A:3861:TRP:CD1	2.51	0.45
1:B:4174:ASP:OD1	1:B:4174:ASP:N	2.47	0.45
1:A:3535:ASP:HA	1:A:3553:ARG:HD2	1.98	0.45
1:B:4086:ILE:HA	1:B:4107:VAL:HA	1.97	0.45
1:B:4209:GLN:OE1	1:B:4211:LYS:NZ	2.38	0.45
1:A:3425:THR:HG22	1:A:3432:VAL:HG22	1.98	0.45
1:A:3382:TYR:OH	1:A:3437:LYS:O	2.28	0.45
1:A:2902:GLY:HA3	1:A:2908:CYS:HA	1.98	0.45
1:A:3225:LEU:HD22	1:A:3256:MET:HE1	1.98	0.45
1:A:3409:LEU:HD11	1:A:3424:TRP:CE2	2.52	0.45
1:A:3648:ARG:NH1	1:A:3661:ASP:O	2.50	0.45
1:A:3307:LYS:HG2	1:A:3308:MET:N	2.32	0.45
1:A:3038:GLN:HB3	1:A:3046:CYS:HB3	1.98	0.45
1:B:4384:ARG:HB3	1:B:4411:TYR:CD1	2.52	0.45
1:A:3213:ASN:HB2	1:A:3224:ILE:HG13	2.00	0.44
1:A:3305:HIS:O	1:A:3481:LEU:HD21	2.17	0.44
1:A:3246:ILE:HG13	1:A:3277:LEU:HD23	1.98	0.44
1:B:4145:GLN:HG3	1:B:4147:ASP:OD1	2.18	0.44
1:A:2956:THR:HA	1:A:2967:CYS:SG	2.58	0.44
1:A:3320:PHE:CD1	1:A:3345:HIS:HB3	2.53	0.44
1:A:3374:ILE:HG12	1:A:3381:LEU:HD12	1.99	0.44
1:A:3892:ARG:NH2	1:A:3896:SER:O	2.51	0.44
1:B:4118:LYS:HG2	1:B:4137:ASP:HA	2.00	0.44
1:A:3300:ASP:OD1	1:A:3304:ARG:N	2.51	0.44
1:A:3354:ASP:HA	1:A:3483:LEU:HD13	2.00	0.44
1:A:2956:THR:OG1	1:A:2965:ARG:NH1	2.51	0.43
1:A:3691:ASN:ND2	1:A:3707:CYS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2961:ARG:NH1	1:A:3671:ASP:OD2	2.50	0.43
1:A:3013:ARG:HG3	1:A:3014:CYS:SG	2.59	0.43
1:A:3382:TYR:HB3	1:A:3415:LEU:HD11	2.01	0.43
1:A:3088:HIS:NE2	1:A:3103:SER:HB2	2.33	0.43
1:B:4123:PRO:HB3	1:B:4125:PHE:CZ	2.54	0.43
1:B:4165:SER:O	1:B:4167:ARG:HG3	2.19	0.43
1:A:3858:GLN:HB2	1:A:3861:TRP:HD1	1.83	0.43
1:A:2931:ASN:HD21	1:A:2966:ARG:NH2	2.18	0.42
1:A:3225:LEU:HD23	1:A:3228:LEU:HD21	2.00	0.42
1:B:4195:ASN:HD22	1:B:4238:ILE:HG21	1.83	0.42
1:B:4343:LEU:HB2	1:B:4354:ALA:HB3	2.01	0.42
1:A:3123:ARG:HB2	1:A:3150:ARG:HH11	1.84	0.42
1:A:3605:ASN:ND2	1:A:3621:CYS:O	2.52	0.42
1:A:3780:CYS:HA	1:A:3792:GLU:OE2	2.19	0.42
1:A:3728:ARG:HD2	1:A:3732:HIS:HA	2.00	0.42
1:A:2909:ARG:HG2	1:A:2911:SER:H	1.85	0.42
1:A:3498:ASP:OD2	1:A:3527:CYS:HB2	2.20	0.42
1:A:3016:ARG:N	1:A:3026:GLU:OE2	2.53	0.42
1:A:2953:THR:HB	1:A:2970:GLN:O	2.19	0.42
1:A:3906:ASN:OD1	1:A:3906:ASN:N	2.53	0.42
1:A:3018:ASN:HB2	1:A:3023:TYR:CE2	2.54	0.42
1:A:3269:HIS:HB2	1:A:3532:TRP:CZ2	2.55	0.42
1:A:3290:ASP:N	1:A:3290:ASP:OD1	2.53	0.42
1:B:4161:SER:HB3	1:B:4168:ILE:HD13	2.02	0.42
1:A:3094:ARG:HD3	1:A:3097:ASN:ND2	2.34	0.41
1:A:3314:VAL:HG21	1:A:3339:TRP:CZ2	2.54	0.41
1:A:3852:LYS:N	1:A:3871:ASP:OD2	2.53	0.41
1:B:4292:GLU:HG3	1:B:4293:LYS:HG3	2.01	0.41
1:A:3123:ARG:HB2	1:A:3150:ARG:NH1	2.35	0.41
1:A:3212:ARG:NH2	1:A:3763:GLU:OE2	2.47	0.41
1:A:3271:LEU:HD11	1:A:3274:ALA:HB2	2.02	0.41
1:A:3317:ASN:O	1:A:3318:ASN:C	2.58	0.41
1:B:4299:GLN:NE2	1:B:4305:GLU:O	2.37	0.41
1:A:1227:PRO:HG2	1:A:1230:MET:HB2	2.03	0.41
1:A:3009:ARG:HG3	1:A:3011:SER:H	1.86	0.41
1:A:3891:PHE:HB3	1:A:3899:VAL:O	2.21	0.41
1:B:4215:ALA:HB2	1:B:4222:ARG:HA	2.03	0.41
1:A:3170:GLU:HB2	1:A:3177:ILE:HG13	2.01	0.41
3:D:1:NAG:H61	3:D:2:NAG:C7	2.50	0.41
1:A:2922:SER:OG	1:A:2924:ASN:OD1	2.22	0.41
1:A:3090:ILE:HD12	1:A:3102:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4106:THR:HB	1:B:4149:LEU:HD22	2.02	0.41
1:A:3750:ASN:O	1:A:3754:GLU:HG3	2.20	0.41
1:A:3321:CYS:SG	1:A:3640:GLY:HA3	2.61	0.41
1:A:3361:ILE:HG22	1:A:3362:ILE:HG12	2.03	0.41
1:A:3788:ASP:N	1:A:3788:ASP:OD1	2.52	0.41
1:A:3353:MET:O	1:A:3483:LEU:HB3	2.20	0.41
1:A:3710:ASN:O	1:A:3714:GLN:HG2	2.20	0.41
1:B:4253:GLU:HB3	1:B:4255:VAL:HG22	2.03	0.41
1:A:3796:GLU:HA	1:A:3796:GLU:OE1	2.21	0.40
1:A:3314:VAL:O	1:A:3315:ASP:CB	2.69	0.40
1:A:3320:PHE:HD2	1:A:3360:VAL:HG21	1.87	0.40
1:A:3427:TRP:CD1	1:A:3452:LYS:HB2	2.55	0.40
1:A:3808:THR:OG1	1:A:3827:ASP:OD2	2.38	0.40
1:A:3890:ARG:HD3	1:A:3900:TYR:HB3	2.03	0.40
1:B:4262:ASP:OD1	1:B:4262:ASP:N	2.54	0.40
1:B:4143:LEU:HD23	1:B:4146:PRO:HG3	2.03	0.40
1:B:4069:TYR:CZ	1:B:4311:LEU:HD11	2.57	0.40
1:B:4204:THR:HG22	1:B:4212:ILE:HA	2.03	0.40
1:A:3463:ARG:HA	1:A:3463:ARG:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1073/4660 (23%)	984 (92%)	87 (8%)	2 (0%)	47 79
1	B	359/4660 (8%)	332 (92%)	26 (7%)	1 (0%)	41 74
2	M	1/5 (20%)	1 (100%)	0	0	100 100
All	All	1433/9325 (15%)	1317 (92%)	113 (8%)	3 (0%)	50 79

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%)	28 57
1	B	320/4089 (8%)	297 (93%)	23 (7%)	14 45
2	M	1/1 (100%)	1 (100%)	0	100 100
All	All	1286/8179 (16%)	1221 (95%)	65 (5%)	27 54

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1233	LEU
1	A	1241	ASP
1	A	1245	ILE
1	A	1268	VAL
1	A	2906	ASN
1	A	2931	ASN
1	A	2941	GLN
1	A	2945	CYS
1	A	2972	TRP
1	A	2981	SER
1	A	2992	MET
1	A	3009	ARG
1	A	3039	PHE
1	A	3069	LEU
1	A	3082	PHE
1	A	3111	CYS
1	A	3165	CYS
1	A	3299	SER
1	A	3354	ASP
1	A	3373	THR

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Mol	Chain	Res	Type
1	A	3395	ASP
1	A	3415	LEU
1	A	3416	THR
1	A	3468	SER
1	A	3505	ARG
1	A	3511	MET
1	A	3514	CYS
1	A	3533	LYS
1	A	3541	SER
1	A	3582	ASP
1	A	3597	GLU
1	A	3608	CYS
1	A	3664	ASP
1	A	3666	SER
1	A	3691	ASN
1	A	3741	CYS
1	A	3842	THR
1	A	3843	TYR
1	A	3881	PHE
1	A	3891	PHE
1	A	3897	ARG
1	A	3923	ARG
1	B	4062	GLU
1	B	4083	GLU
1	B	4084	GLU
1	B	4090	ASP
1	B	4108	LEU
1	B	4110	GLN
1	B	4130	ASN
1	B	4144	MET
1	B	4147	ASP
1	B	4160	TRP
1	B	4164	LYS
1	B	4179	LYS
1	B	4188	GLN
1	B	4194	VAL
1	B	4217	MET
1	B	4246	VAL
1	B	4268	LEU
1	B	4279	LEU
1	B	4311	LEU
1	B	4313	VAL

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Mol	Chain	Res	Type
1	B	4375	LEU
1	B	4387	HIS
1	B	4414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2906	ASN
1	A	2931	ASN
1	A	2943	HIS
1	A	3679	ASN
1	A	3714	GLN
1	A	3782	GLN
1	B	4145	GLN
1	B	4387	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)

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	0.51	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	C	3	3	11,11,12	0.26	0	15,15,17	0.74	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	0.89	0
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.64	0
4	NAG	E	1	4,1	14,14,15	0.31	0	17,19,21	0.67	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.72	0
4	BMA	E	3	4	11,11,12	0.28	0	15,15,17	1.03	1 (6%)
4	MAN	E	4	4	11,11,12	0.25	0	15,15,17	0.77	0
4	MAN	E	5	4	11,11,12	0.21	0	15,15,17	0.75	0
5	NAG	F	1	1,5	14,14,15	0.26	0	17,19,21	0.73	0
5	NAG	F	2	5	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	G	1	1,5	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	G	2	5	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	H	1	4,1	14,14,15	0.31	0	17,19,21	0.92	0
4	NAG	H	2	4	14,14,15	0.32	0	17,19,21	0.61	0
4	BMA	H	3	4	11,11,12	0.25	0	15,15,17	0.89	1 (6%)
4	MAN	H	4	4	11,11,12	0.22	0	15,15,17	0.69	0
4	MAN	H	5	4	11,11,12	0.22	0	15,15,17	0.72	0
4	NAG	I	1	4,1	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.72	0
4	BMA	I	3	4	11,11,12	0.23	0	15,15,17	0.85	0
4	MAN	I	4	4	11,11,12	0.24	0	15,15,17	0.68	0
4	MAN	I	5	4	11,11,12	0.23	0	15,15,17	0.65	0
5	NAG	J	1	5	14,14,15	0.28	0	17,19,21	0.50	0
5	NAG	J	2	5	14,14,15	0.31	0	17,19,21	0.73	0
6	NAG	K	1	6	14,14,15	0.27	0	17,19,21	0.57	0
6	NAG	K	2	6	14,14,15	0.31	0	17,19,21	0.65	0
6	BMA	K	3	6	11,11,12	0.23	0	15,15,17	0.74	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	-	0/6/23/26	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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4,1	-	4/6/23/26	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	-	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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	3	BMA	C1-C2-C3	2.49	112.72	109.67
4	I	1	NAG	C1-O5-C5	2.47	115.54	112.19
4	H	3	BMA	C1-O5-C5	2.33	115.34	112.19
3	D	1	NAG	C2-N2-C7	-2.12	119.88	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
6	K	3	BMA	O5-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	3	BMA	O5-C5-C6-O6
4	H	1	NAG	C3-C2-N2-C7
5	G	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O7-C7-N2-C2

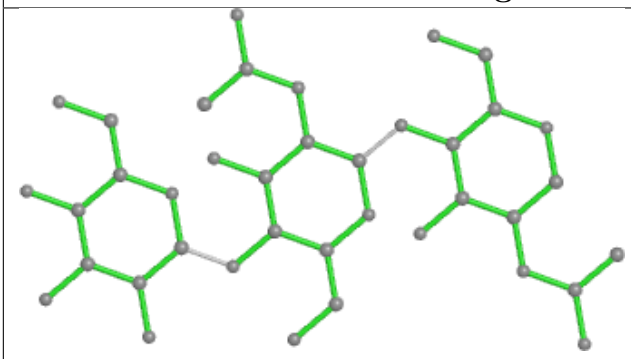
There are no ring outliers.

2 monomers are involved in 1 short contact:

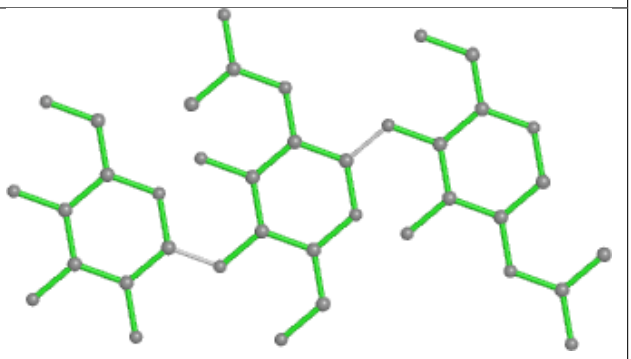
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	D	1	NAG	1	0

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

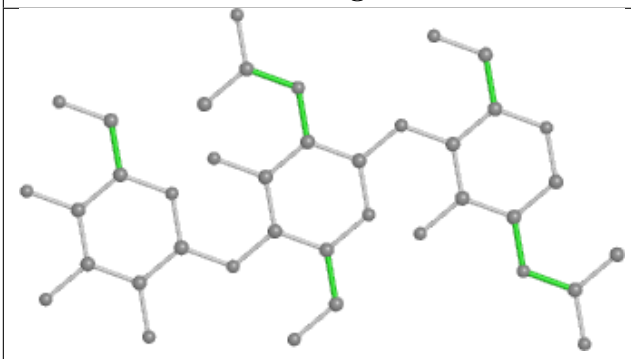
Oligosaccharide Chain C



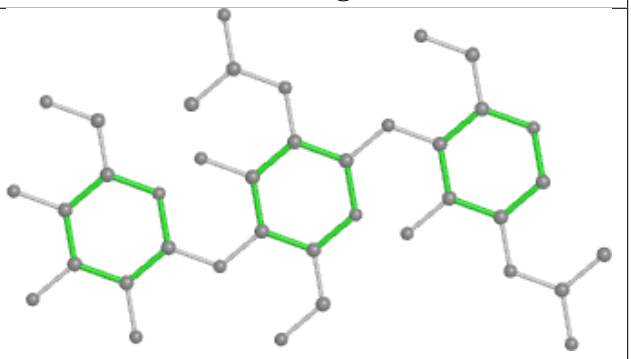
Bond lengths



Bond angles

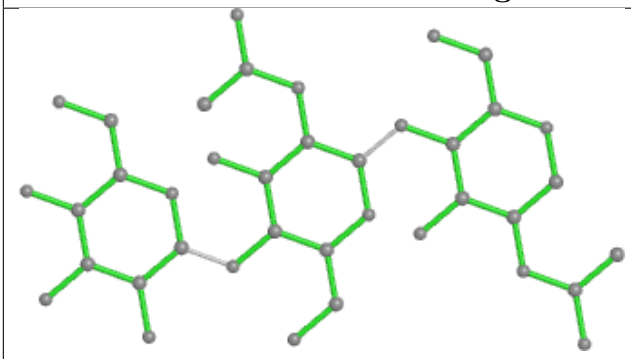


Torsions

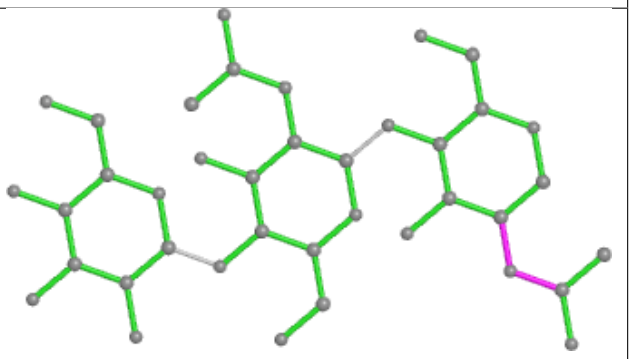


Rings

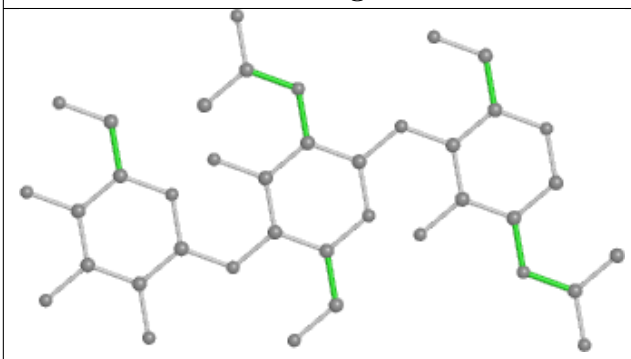
Oligosaccharide Chain D



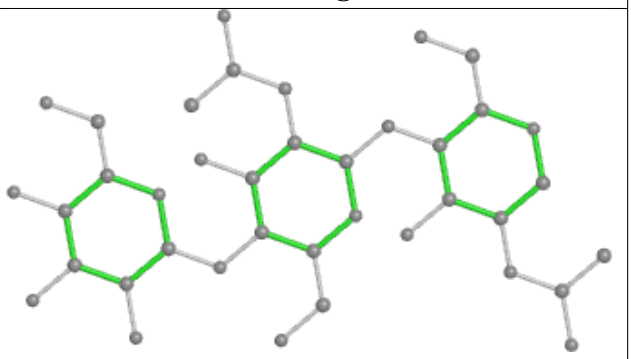
Bond lengths



Bond angles

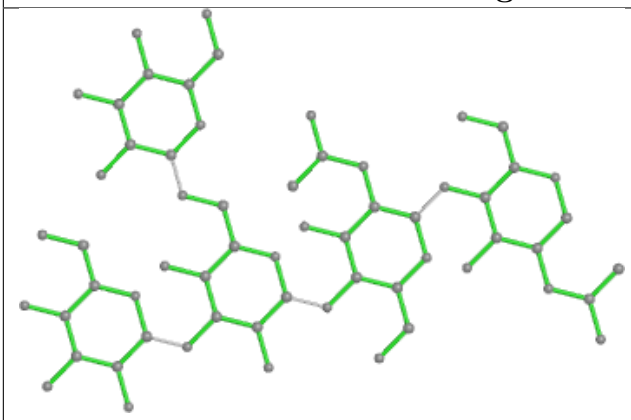


Torsions

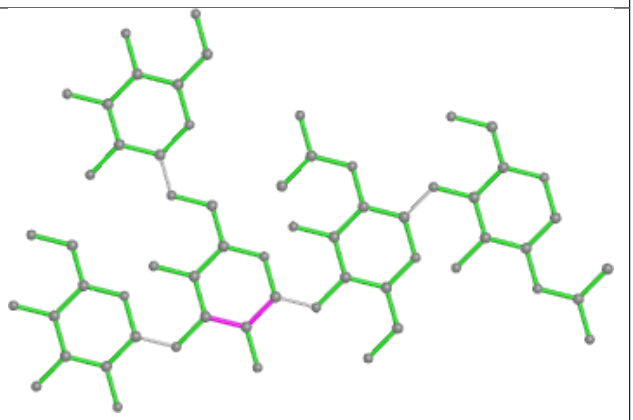


Rings

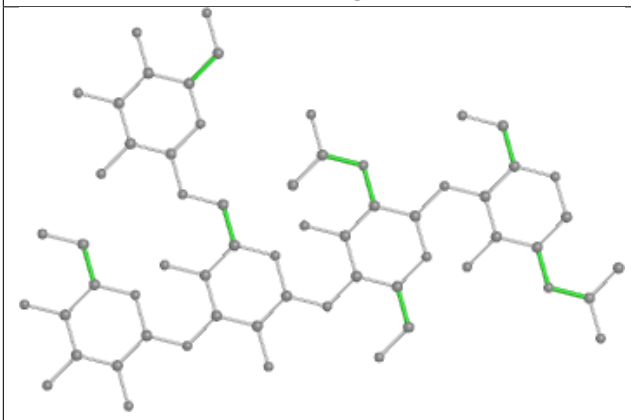
Oligosaccharide Chain E



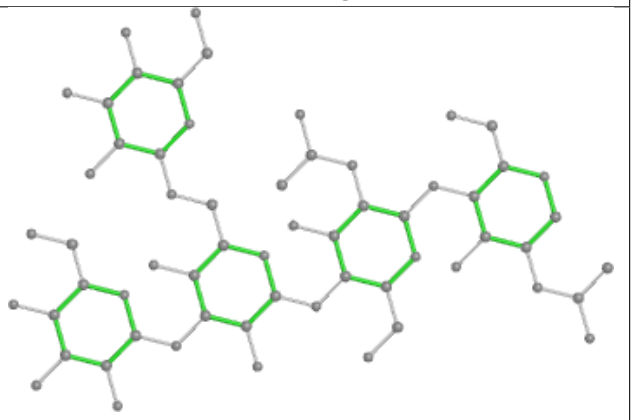
Bond lengths



Bond angles

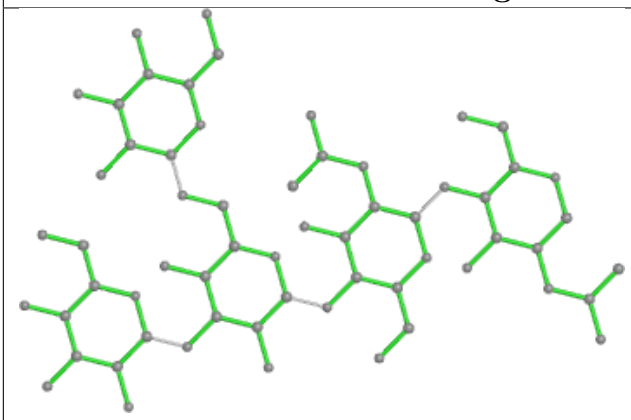


Torsions

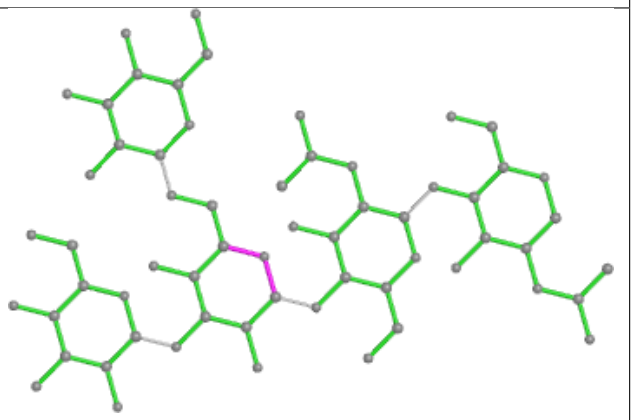


Rings

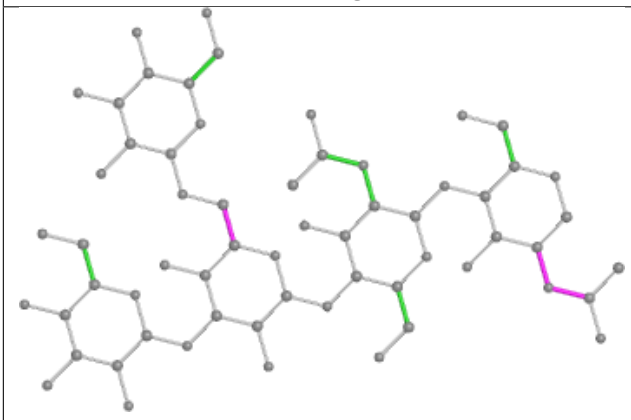
Oligosaccharide Chain H



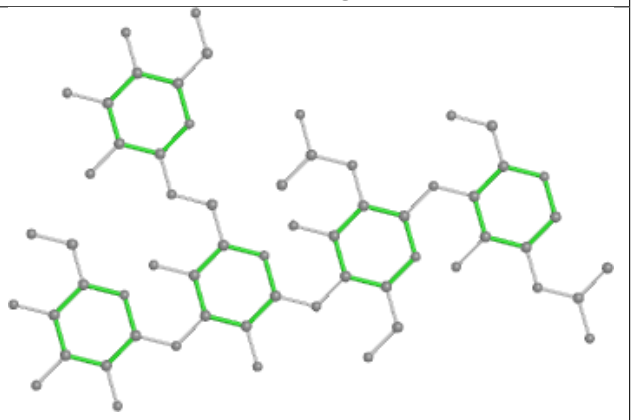
Bond lengths



Bond angles

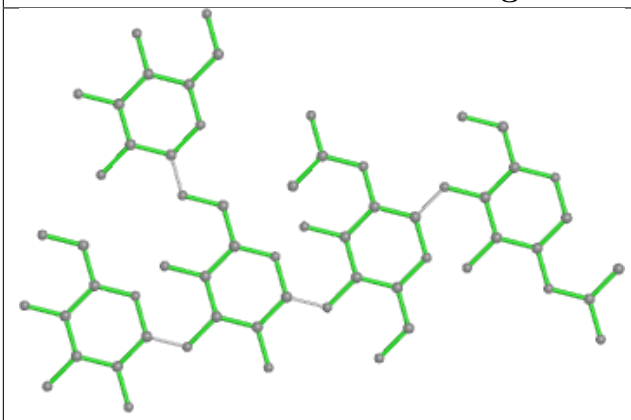


Torsions

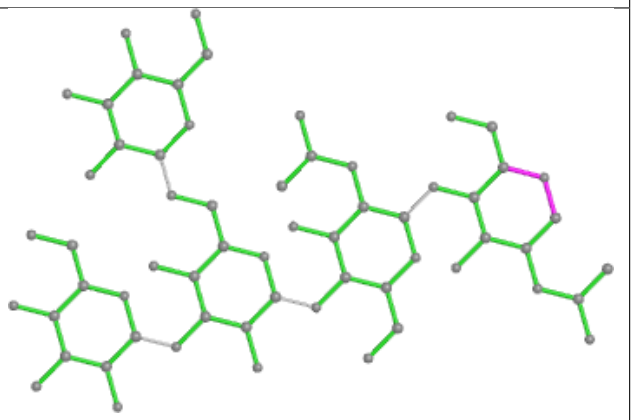


Rings

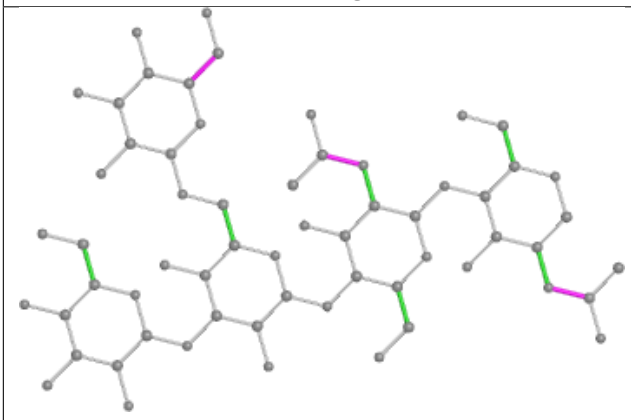
Oligosaccharide Chain I



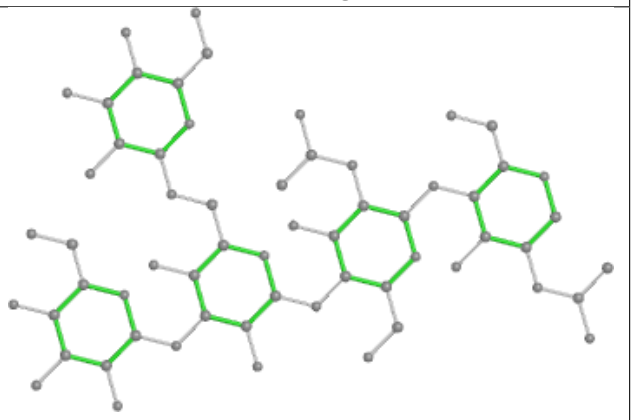
Bond lengths



Bond angles

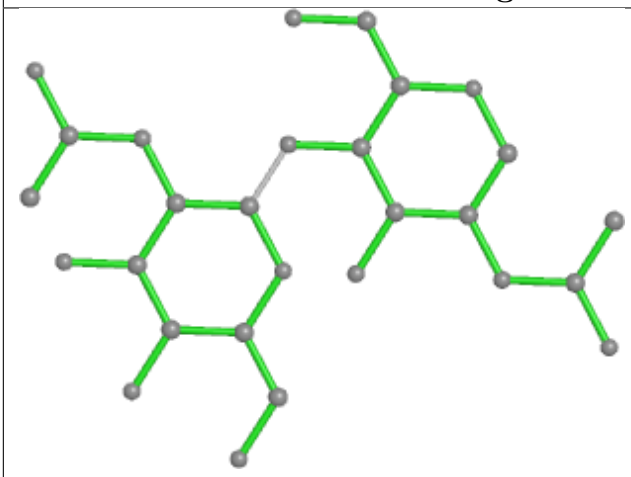


Torsions

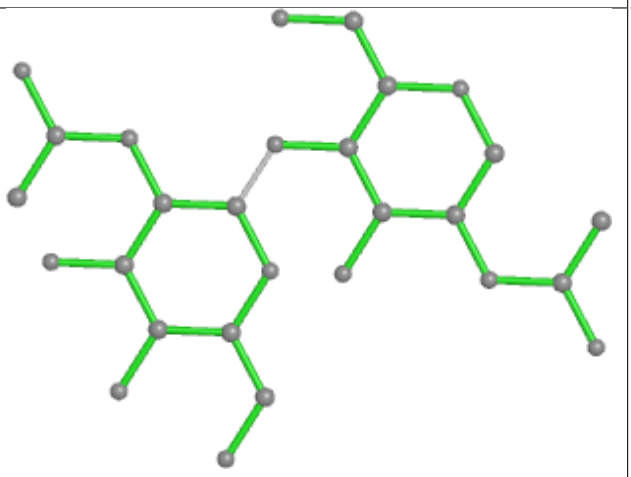


Rings

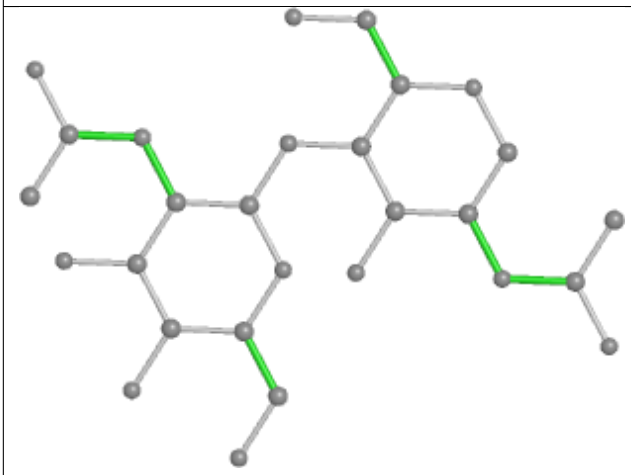
Oligosaccharide Chain F



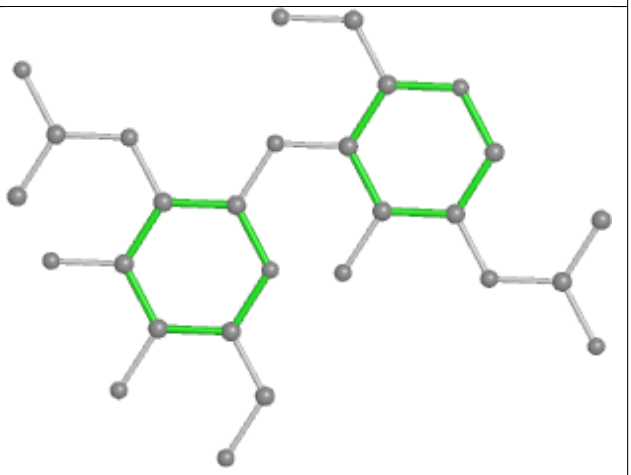
Bond lengths



Bond angles

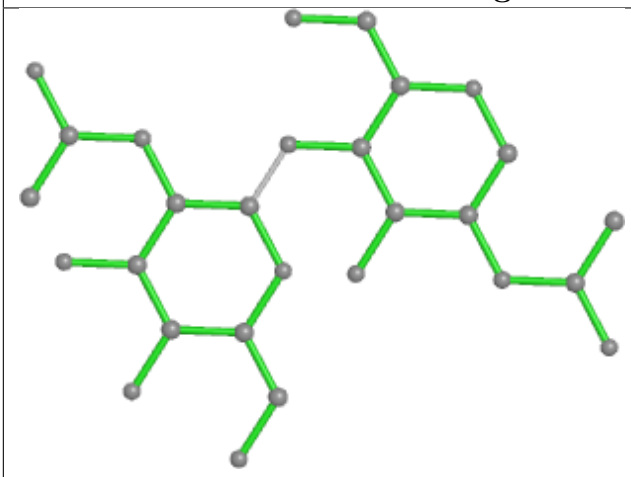


Torsions

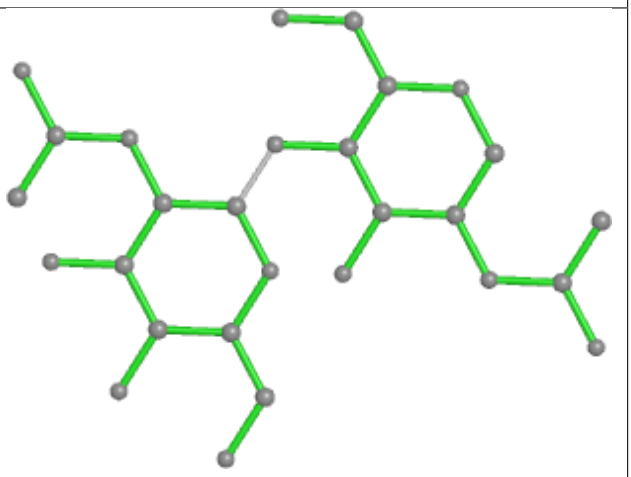


Rings

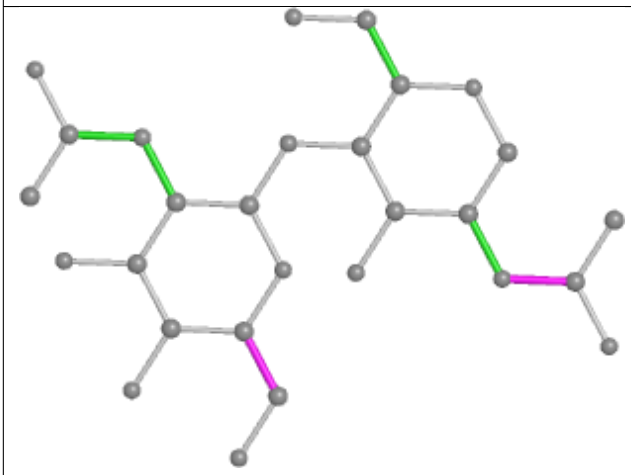
Oligosaccharide Chain G



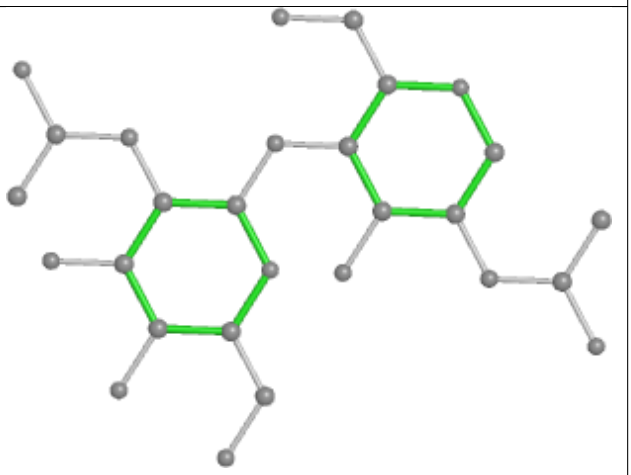
Bond lengths



Bond angles

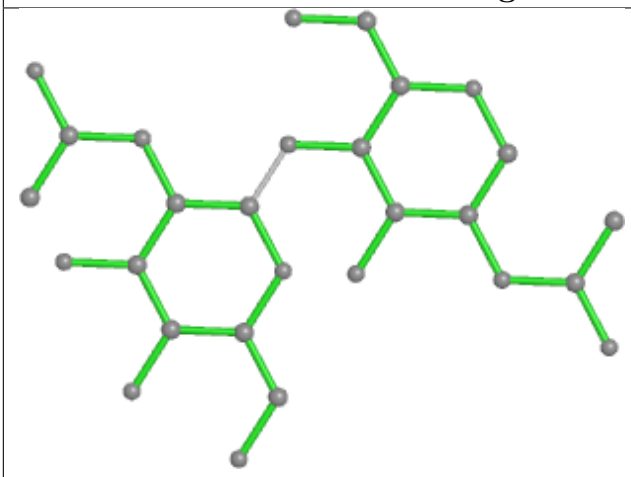


Torsions

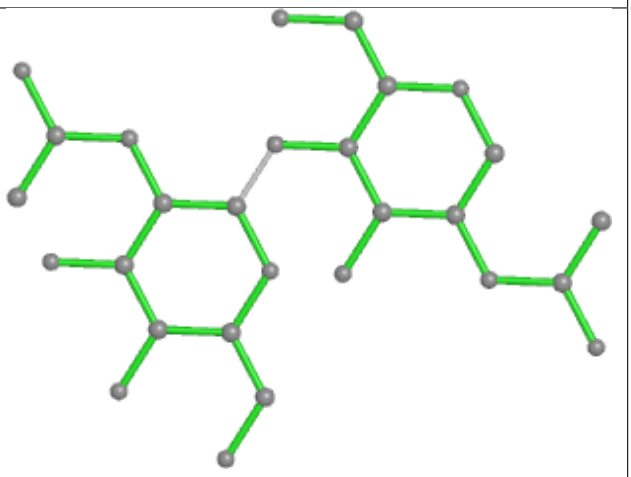


Rings

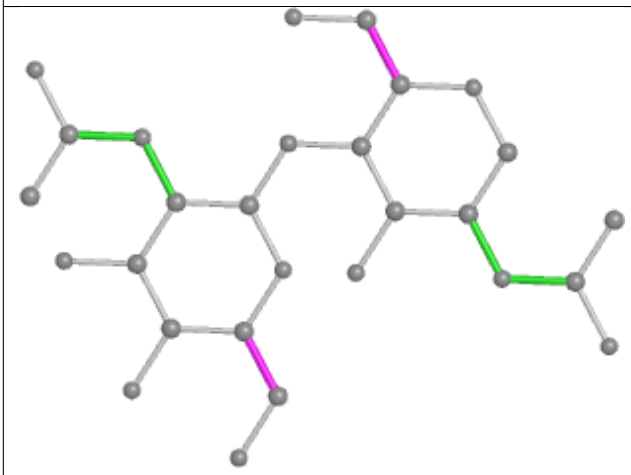
Oligosaccharide Chain J



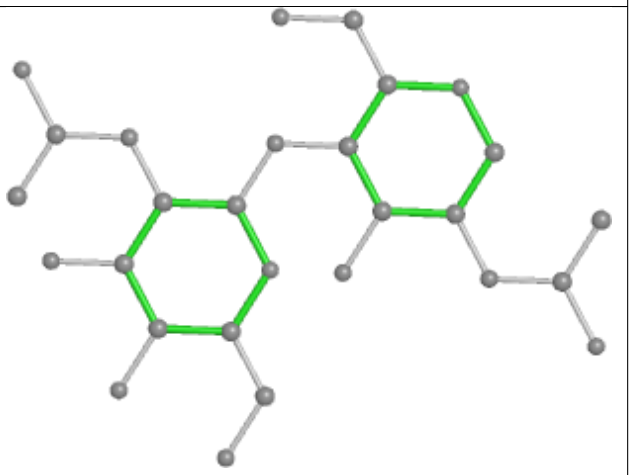
Bond lengths



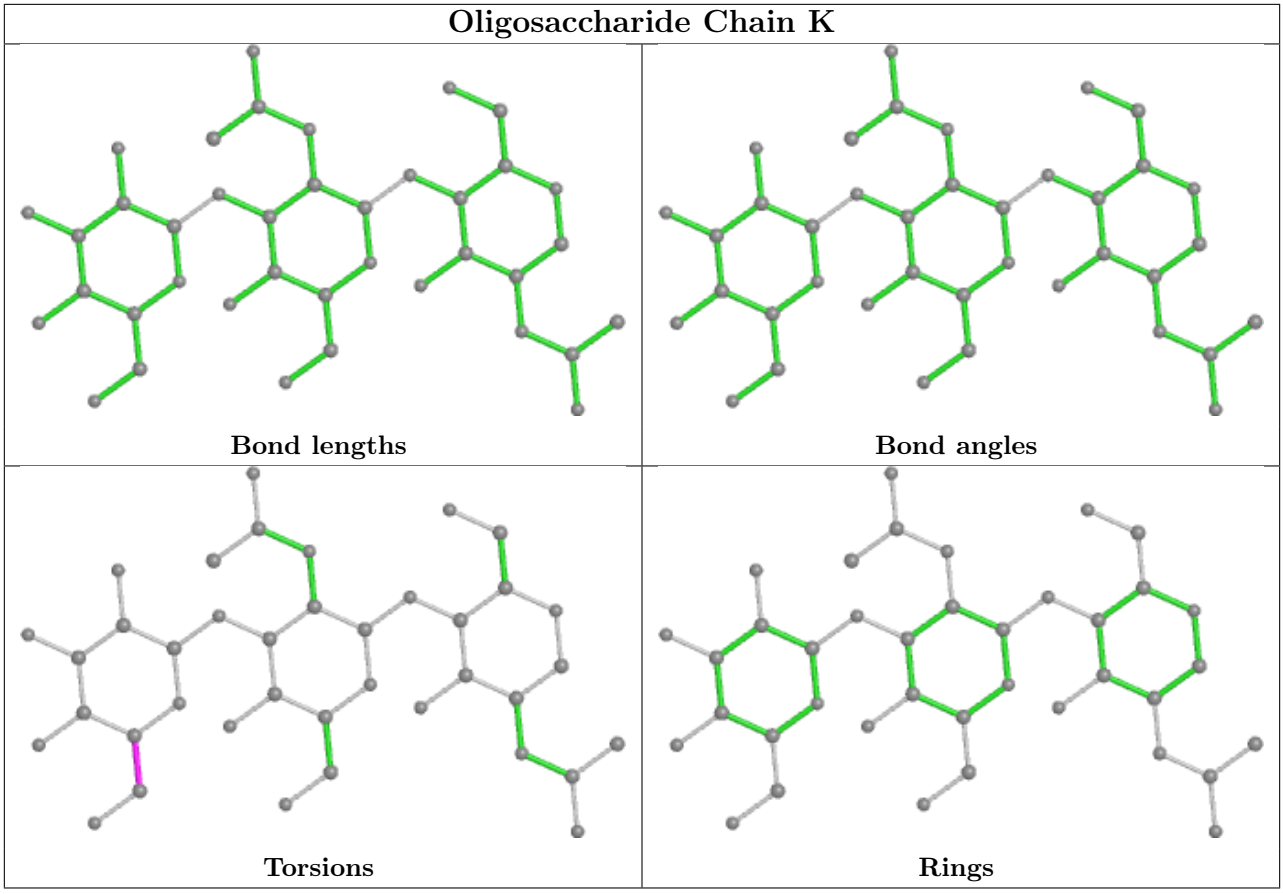
Bond angles



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	$\#\|Z\| > 2$
8	A2G	A	4705	1	14,14,15	0.41	0	17,19,21	0.53	0
8	A2G	A	4706	1	14,14,15	0.39	0	17,19,21	0.61	0
8	A2G	A	4707	1	14,14,15	0.39	0	17,19,21	0.57	0
8	A2G	A	4704	1	14,14,15	0.40	0	17,19,21	0.67	0
8	A2G	A	4703	1	14,14,15	0.40	0	17,19,21	0.69	0
7	NAG	A	4702	1	14,14,15	0.26	0	17,19,21	0.65	0
7	NAG	A	4701	1	14,14,15	0.30	0	17,19,21	0.60	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
8	A2G	A	4705	1	-	2/6/23/26	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	4703	1	-	0/6/23/26	0/1/1/1
7	NAG	A	4702	1	-	3/6/23/26	0/1/1/1
7	NAG	A	4701	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4702	NAG	C8-C7-N2-C2
7	A	4702	NAG	O7-C7-N2-C2
7	A	4702	NAG	C1-C2-N2-C7
8	A	4705	A2G	C1-C2-N2-C7
8	A	4707	A2G	O5-C5-C6-O6
7	A	4701	NAG	C1-C2-N2-C7
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.

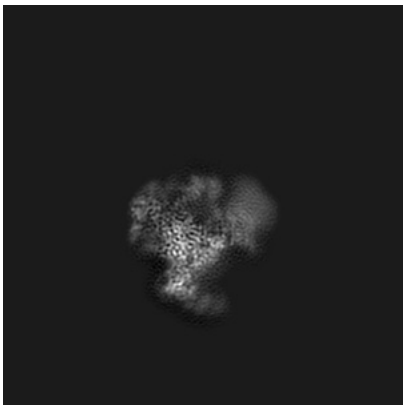
6 Map visualisation

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.

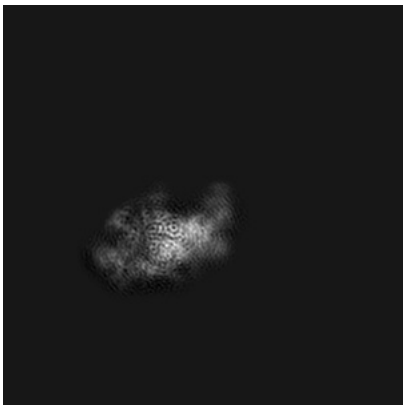
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

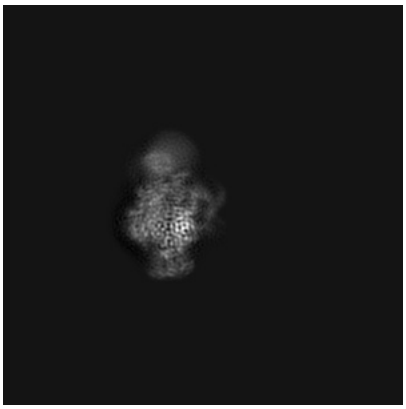
6.1.1 Primary map



X

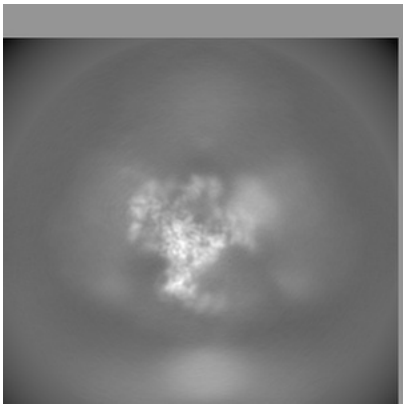


Y

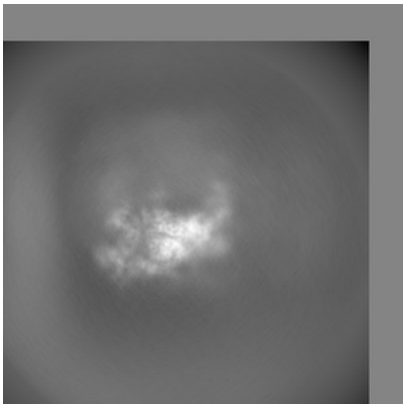


Z

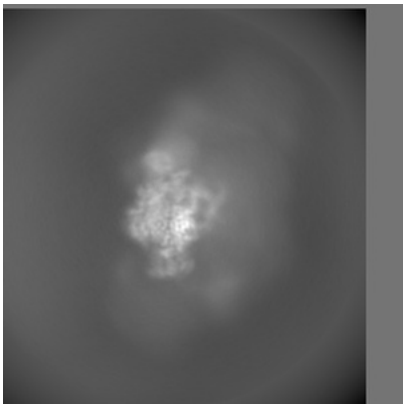
6.1.2 Raw map



X



Y

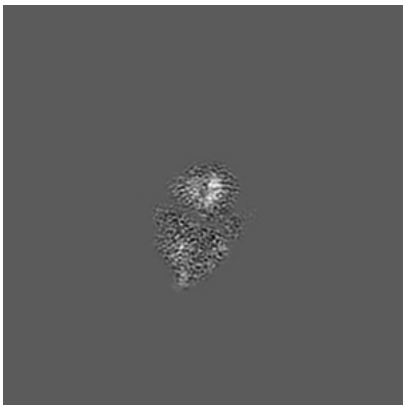


Z

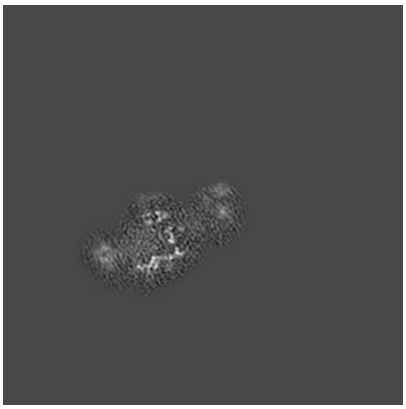
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

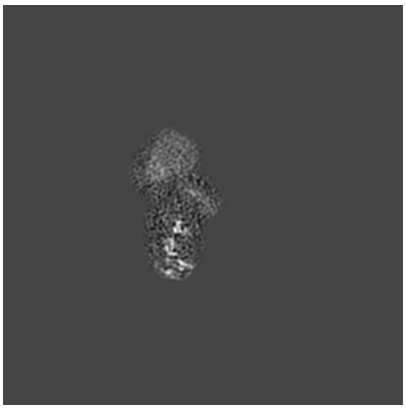
6.2.1 Primary map



X Index: 130

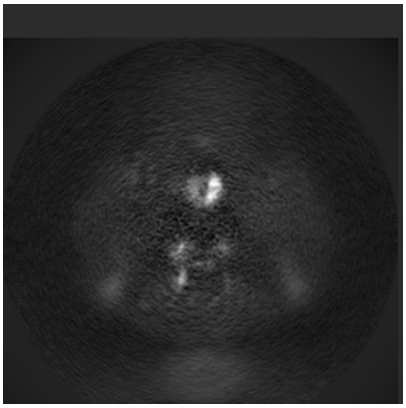


Y Index: 130

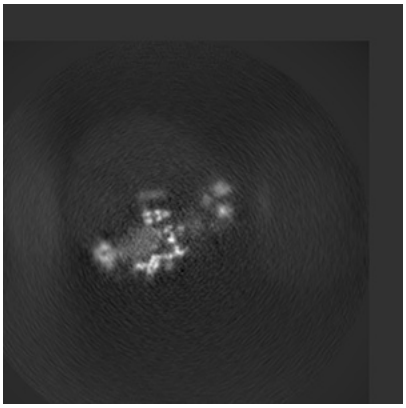


Z Index: 130

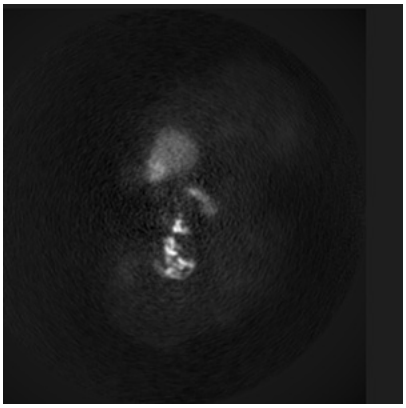
6.2.2 Raw map



X Index: 130



Y Index: 130

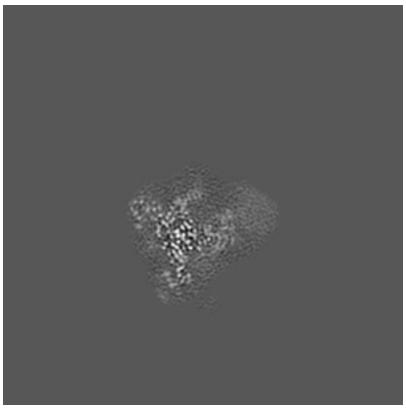


Z Index: 130

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

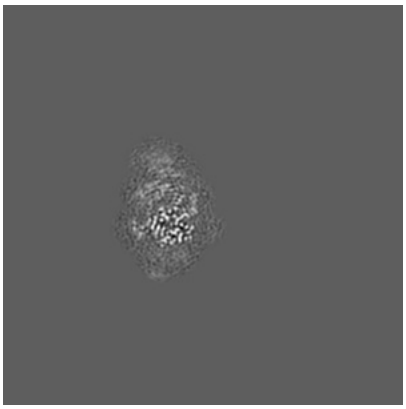
6.3 Largest variance slices (i)

6.3.1 Primary map



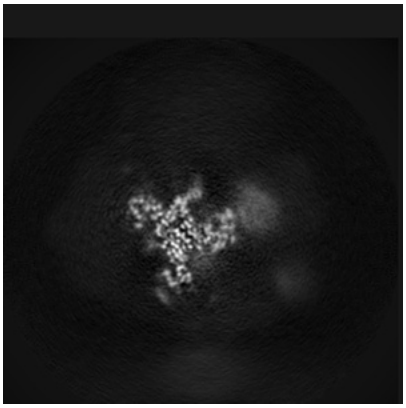
X Index: 113

Y Index: 115

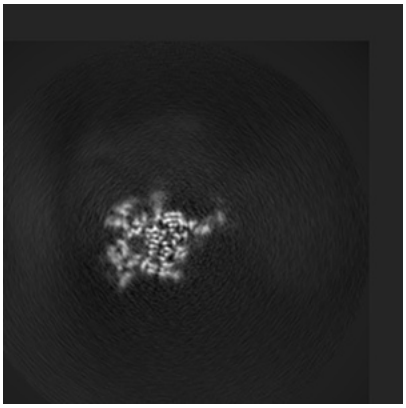


Z Index: 106

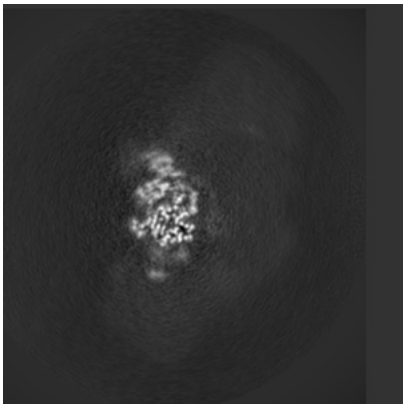
6.3.2 Raw map



X Index: 113



Y Index: 115

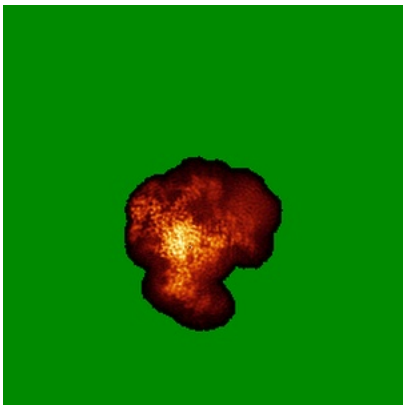


Z Index: 106

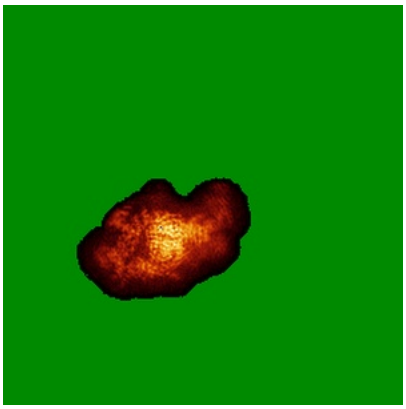
The images above show the largest variance slices of the map in three orthogonal directions.

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

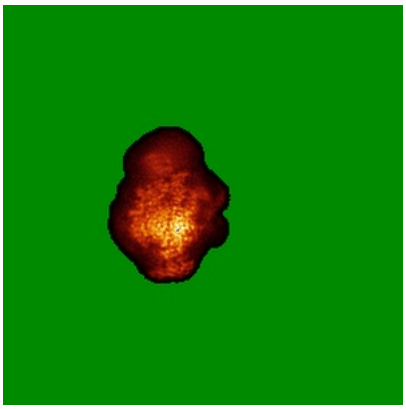
6.4.1 Primary map



X

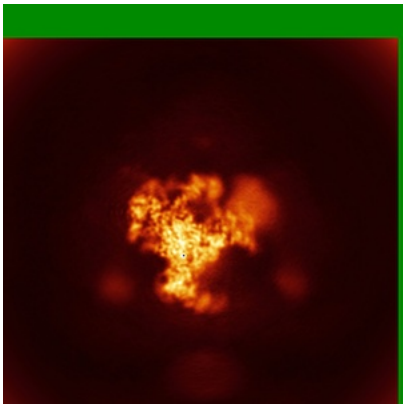


Y

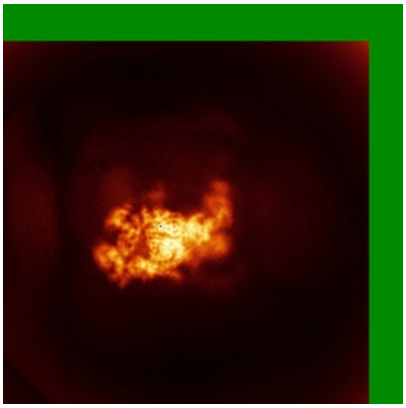


Z

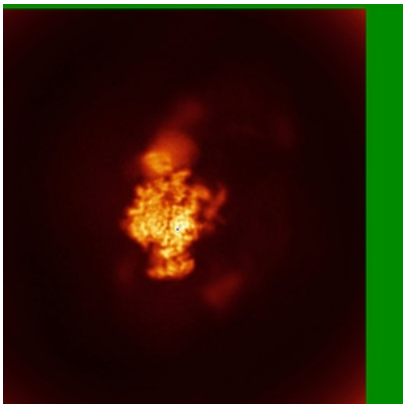
6.4.2 Raw map



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.

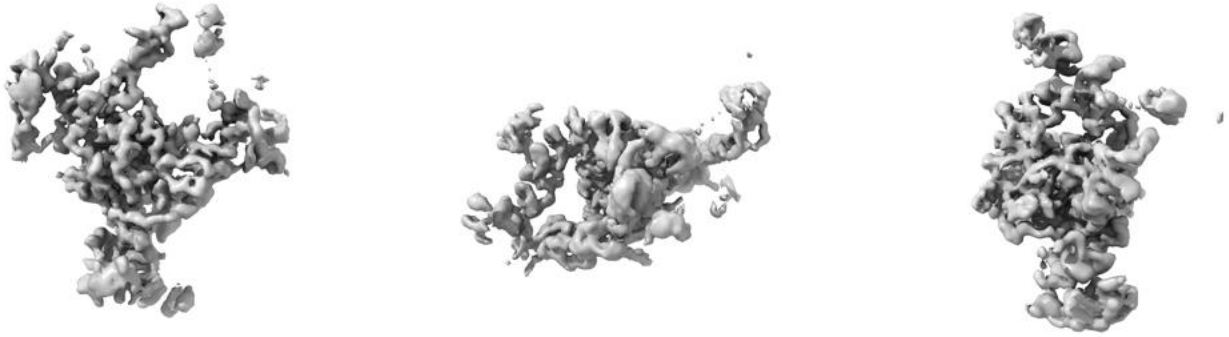
6.5 Orthogonal surface views (i)

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.

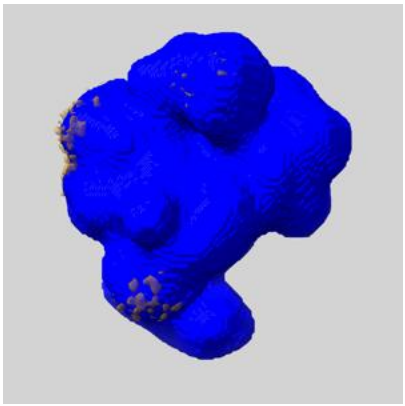
6.6 Mask visualisation (i)

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

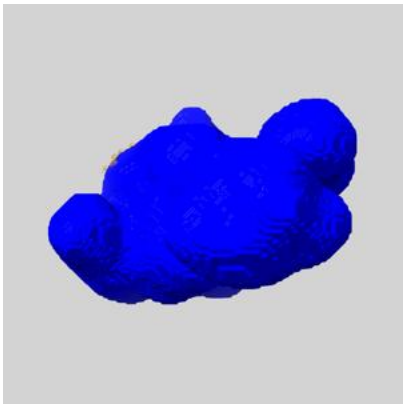
A mask typically either:

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

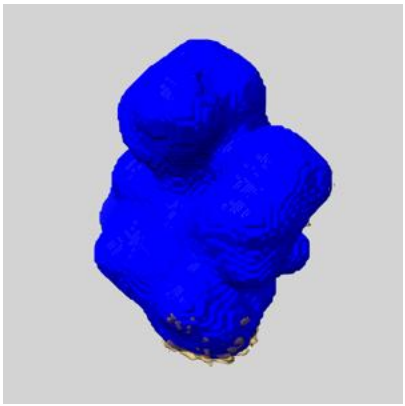
6.6.1 emd_36694_msk_1.map (i)



X



Y

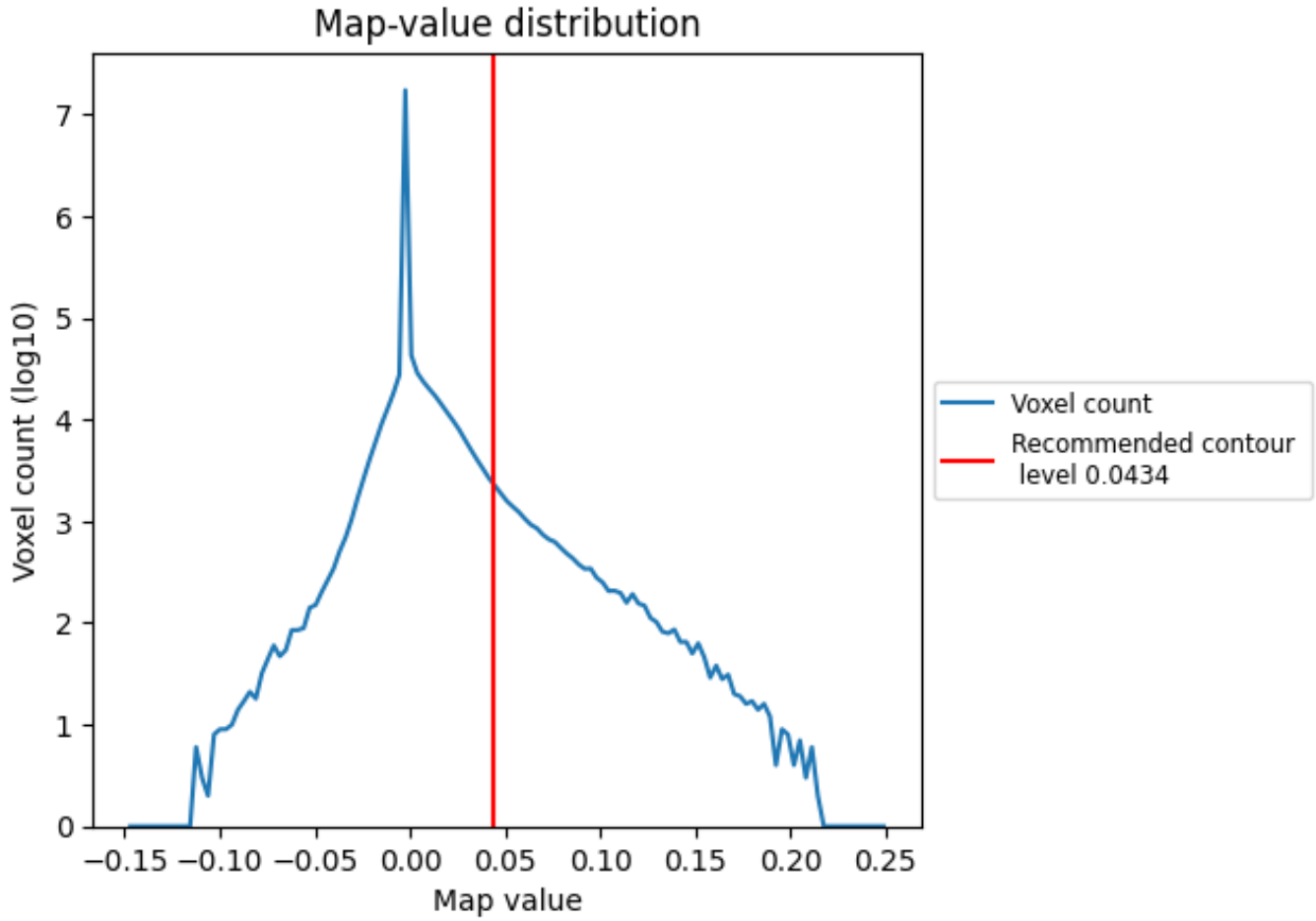


Z

7 Map analysis

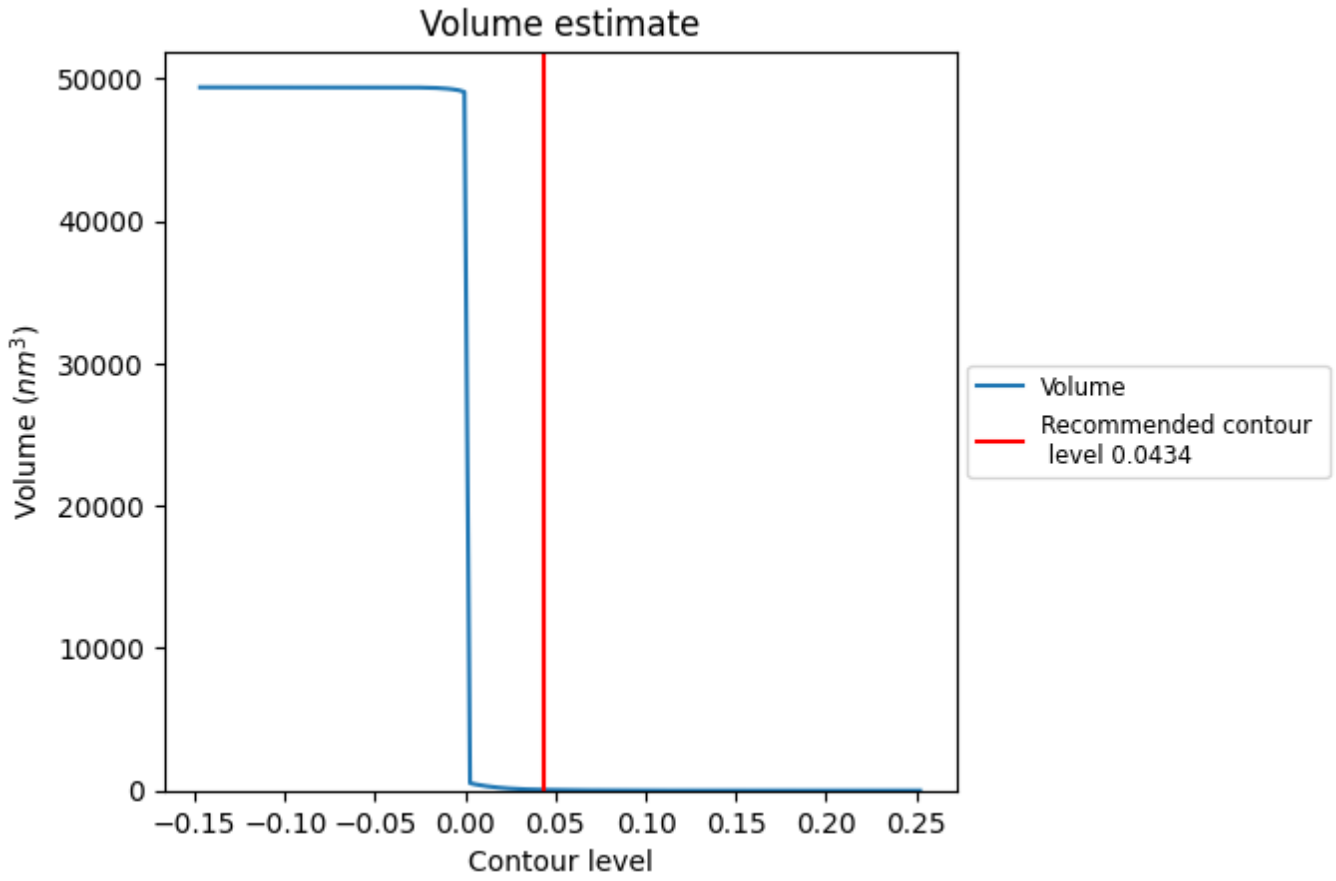
This section contains the results of statistical analysis of the map.

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.

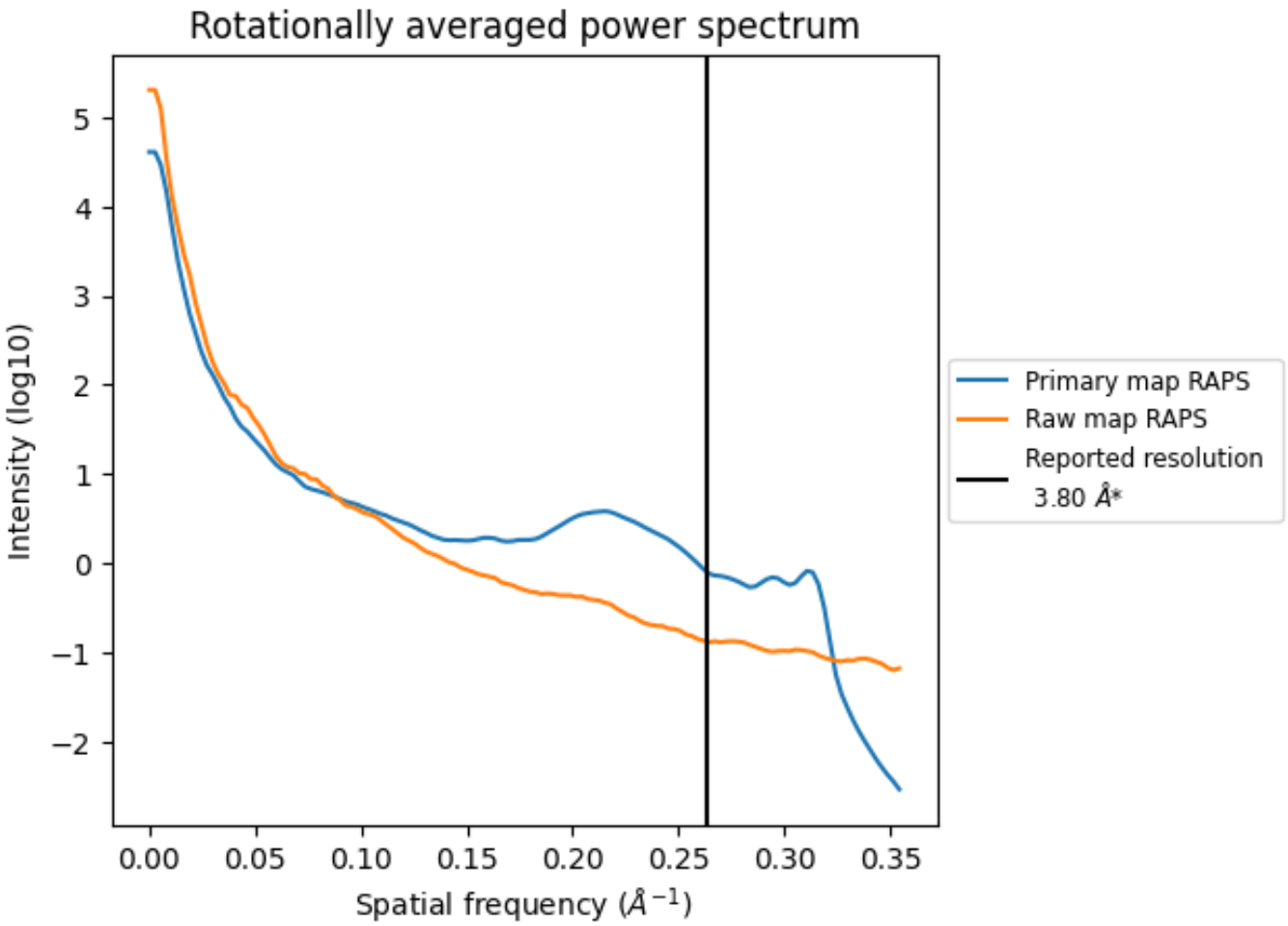
7.2 Volume estimate



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)

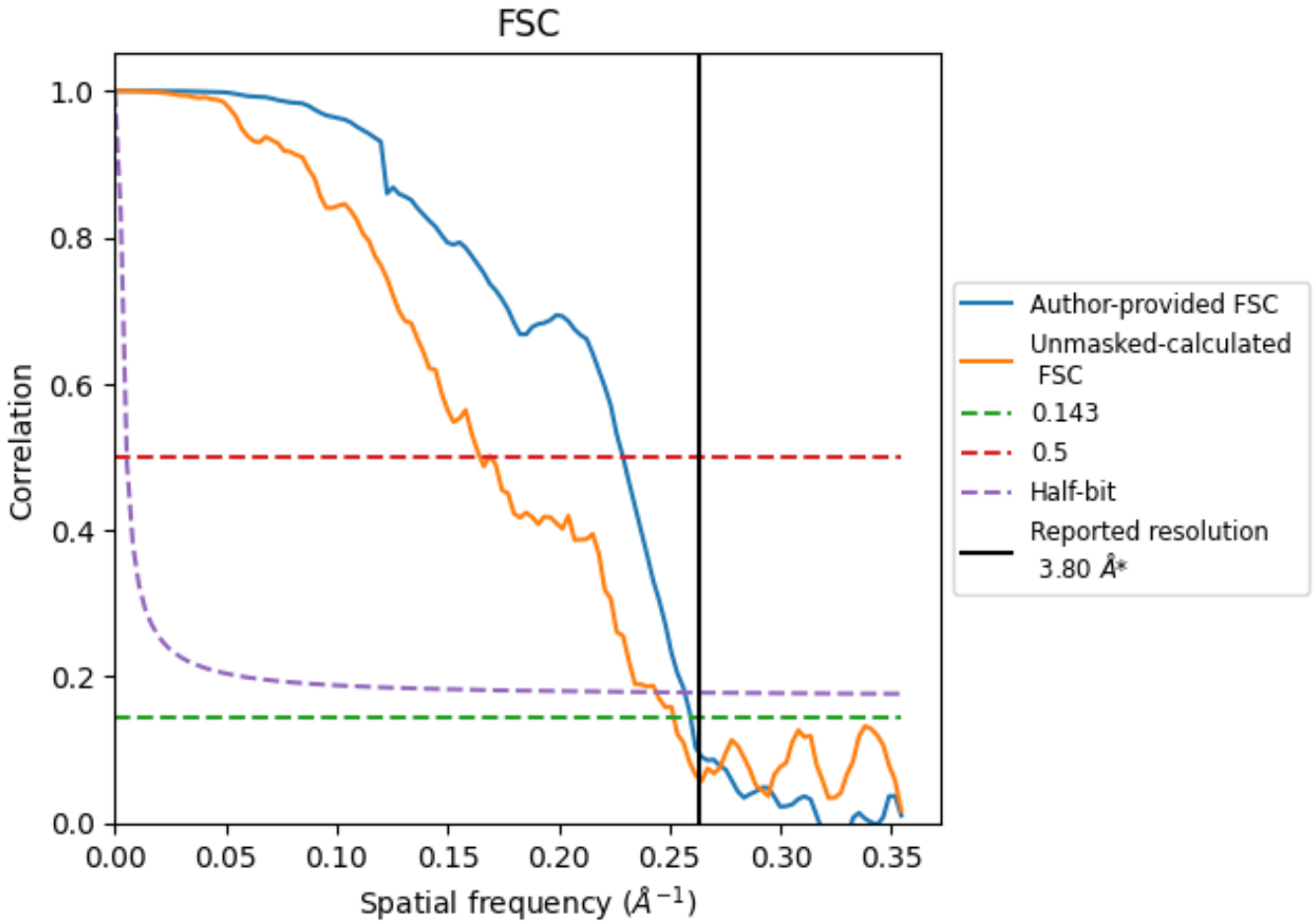


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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)

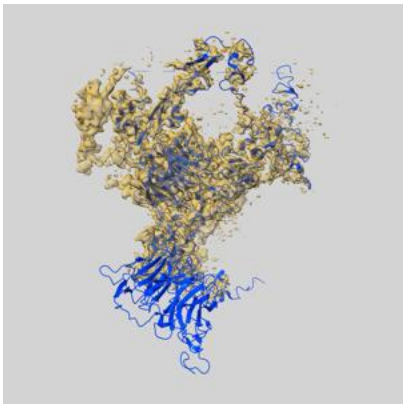
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.86	4.37	3.89
Unmasked-calculated*	3.97	6.08	4.10

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

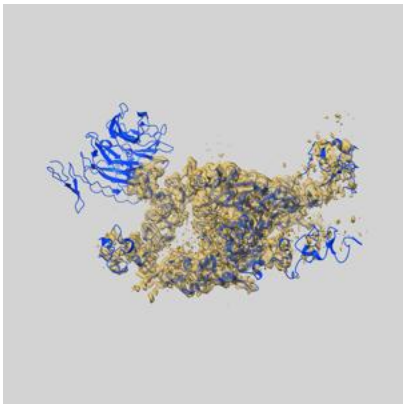
9 Map-model fit

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.

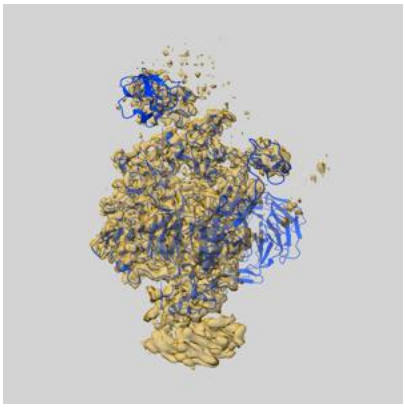
9.1 Map-model overlay



X



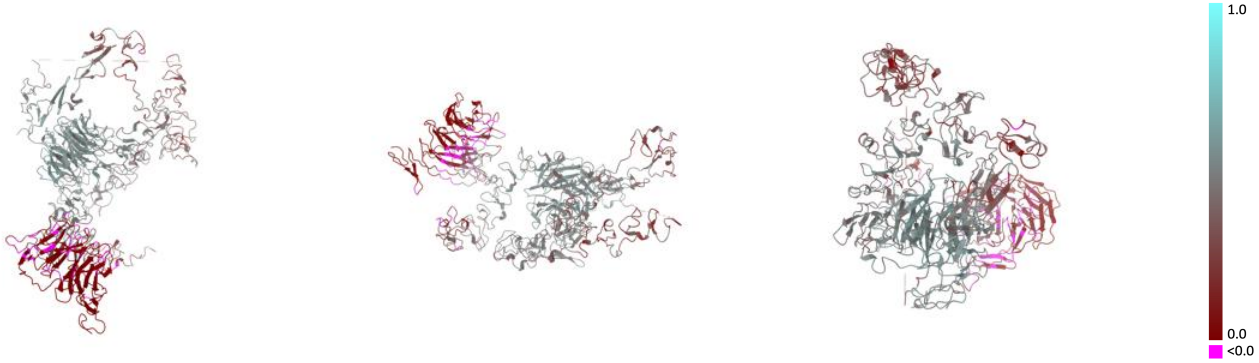
Y



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.

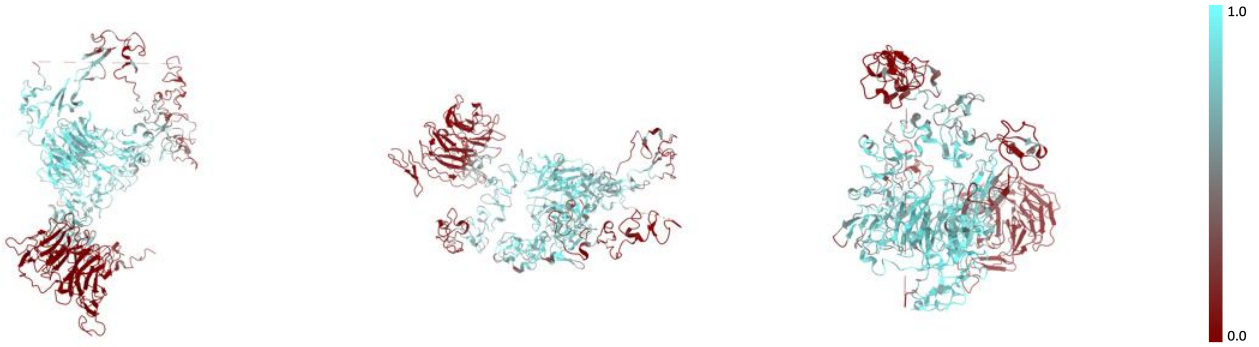
9.2 Q-score mapped to coordinate model (i)



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.

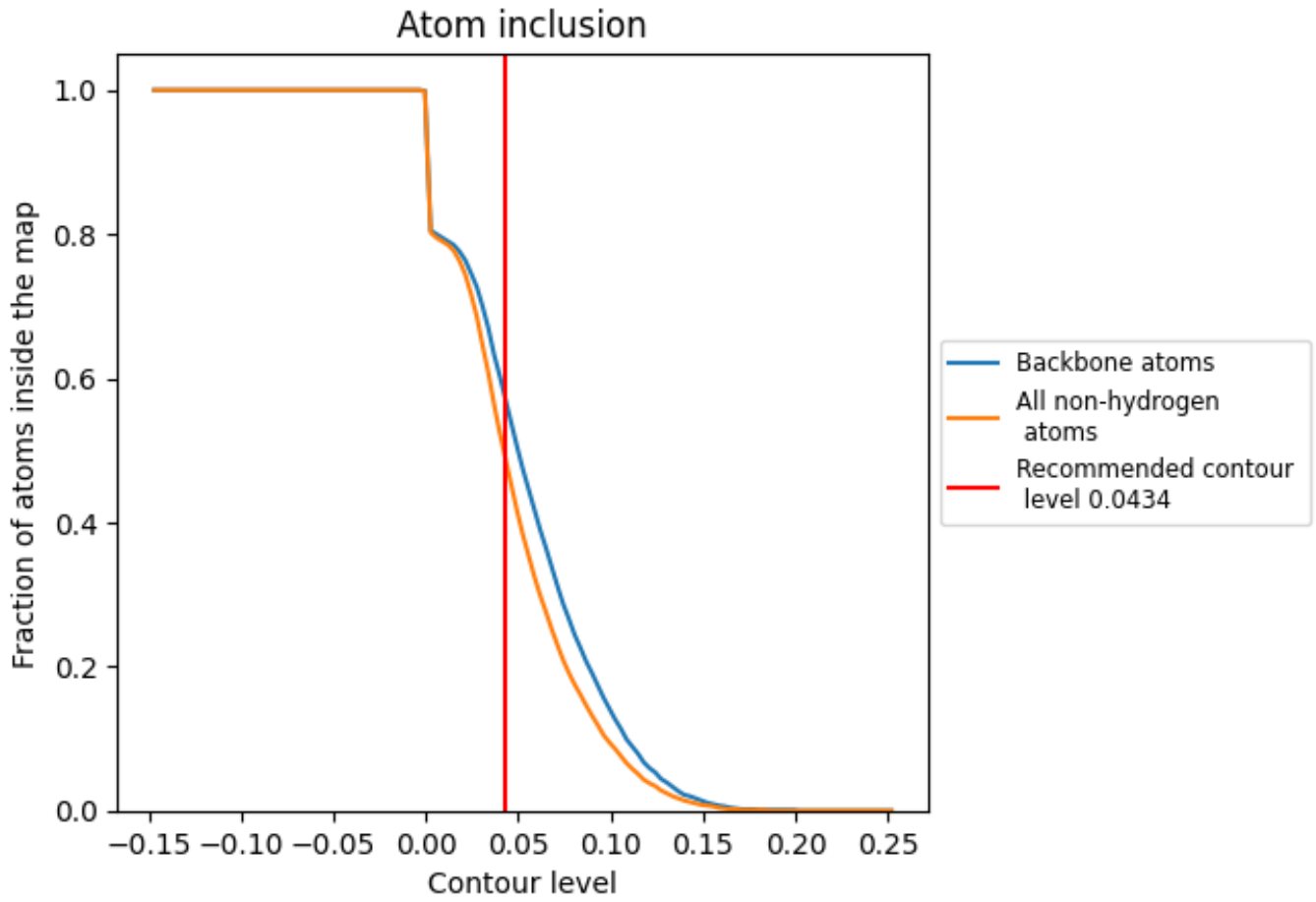
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0434).

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