wwPDB EM Validation Summary Report

Oct 27, 2024 – 12:53 PM JST

PDB ID	:	6JK8
EMDB ID	:	EMD-9838
Title	:	Cryo-EM structure of the full-length human IGF-1R in complex with insulin
Authors	:	Zhang, X.; Yu, D.; Wang, T.
Deposited on	:	2019-02-27
Resolution	:	5.00 Å(reported)

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

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

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

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

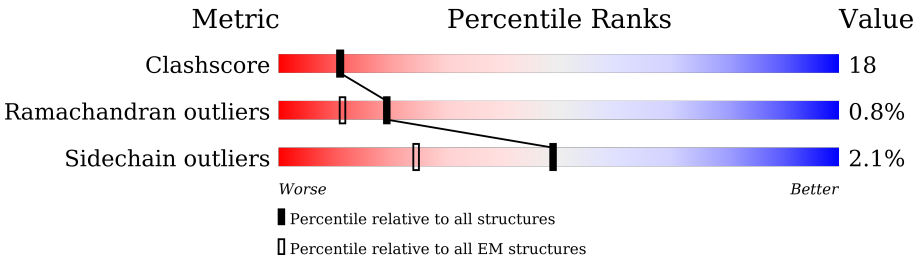
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 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	1367	24% 35% 23% • 40%
1	B	1367	26% 33% 24% • 41%
2	C	110	11% 8% 10% • 81%
2	D	110	11% 13% 5% • • 77%
3	E	2	100%
3	G	2	50% 50% 50%
3	H	2	50% 50% 50%
3	I	2	100%

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Mol	Chain	Length	Quality of chain
4	F	4	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13666 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	823	Total 6595	C 4166	N 1138	O 1241	S 50	0	0
1	B	801	Total 6450	C 4076	N 1119	O 1209	S 46	1	0

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	21	Total 163	C 99	N 25	O 35	S 4	0	0
2	D	25	Total 212	C 138	N 35	O 37	S 2	1	0

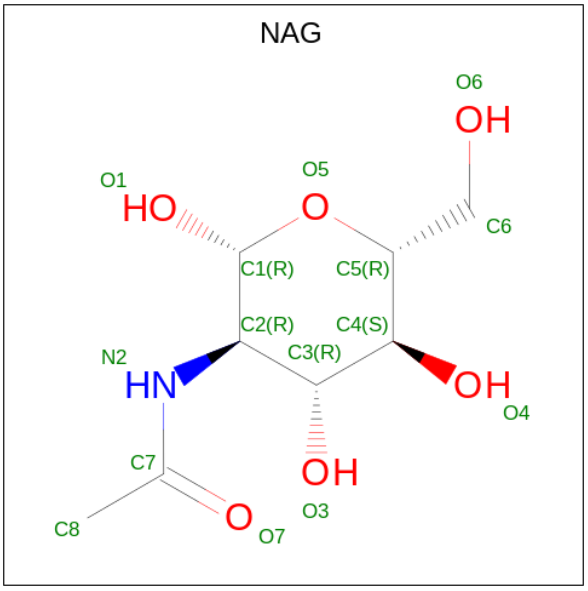
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-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	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



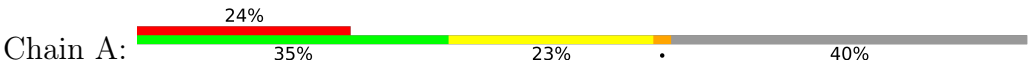
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

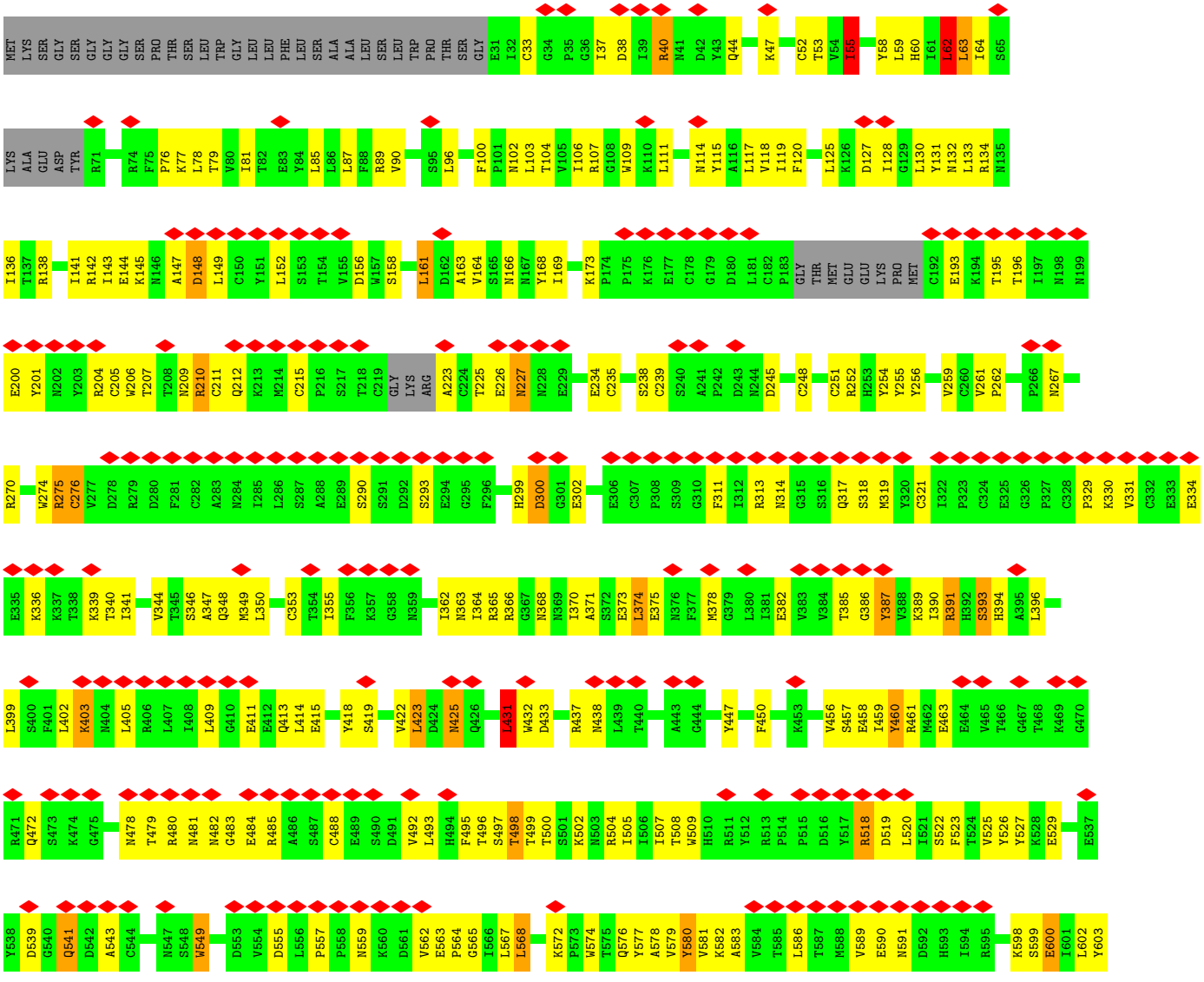
3 Residue-property plots (i)

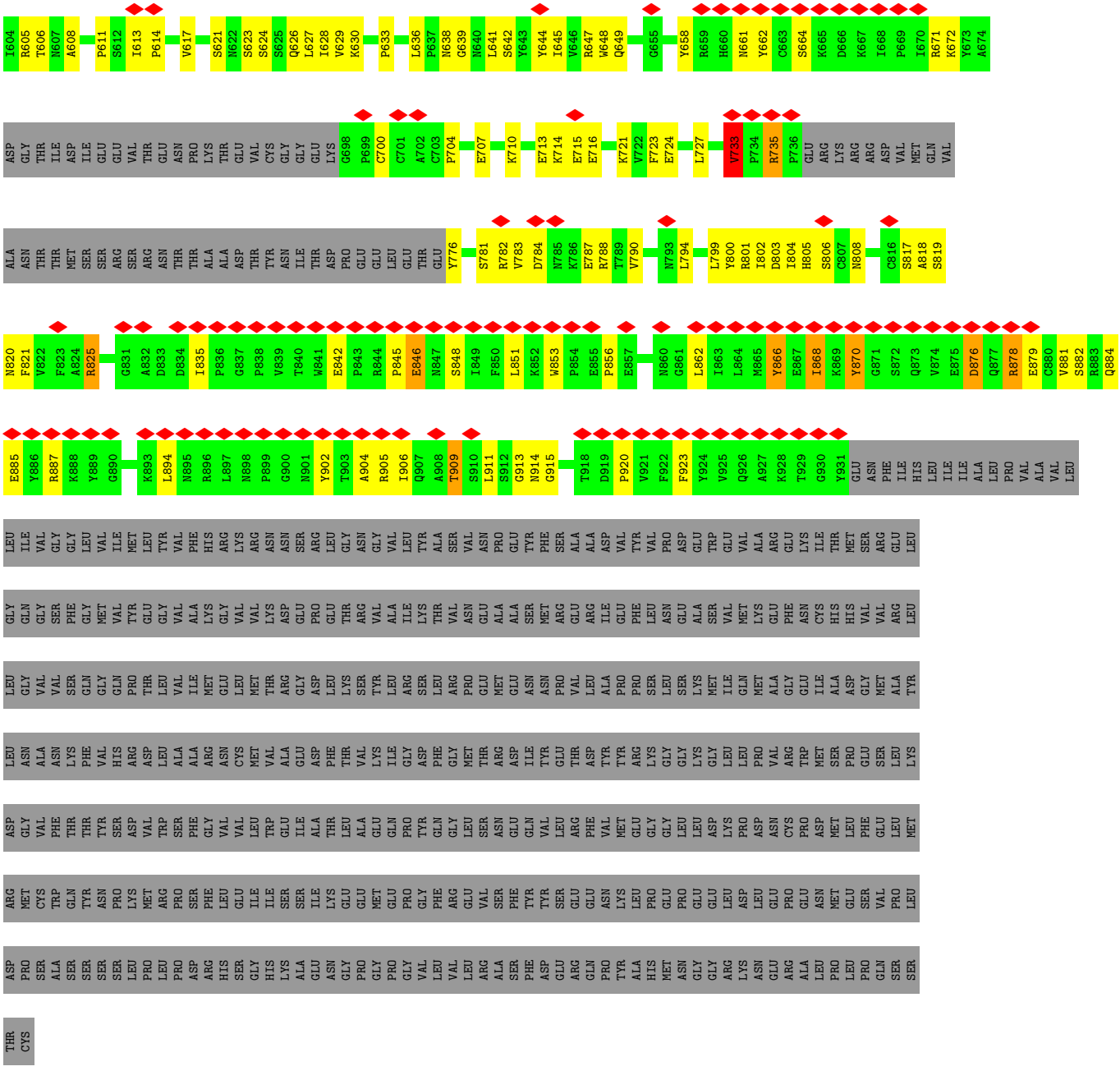
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Insulin-like growth factor 1 receptor

Chain A:

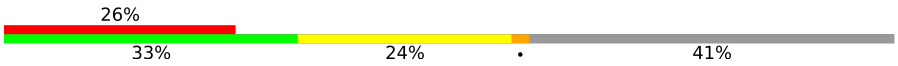


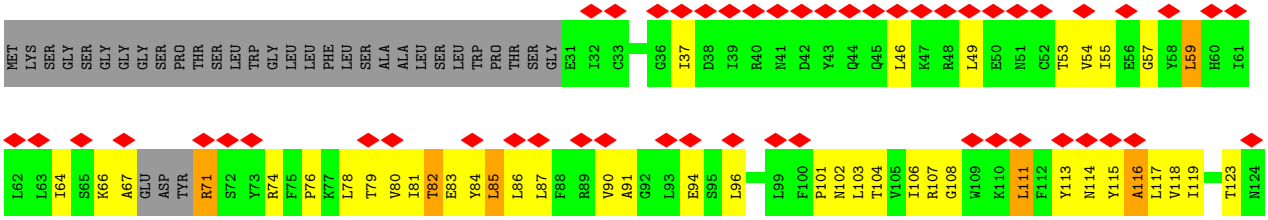


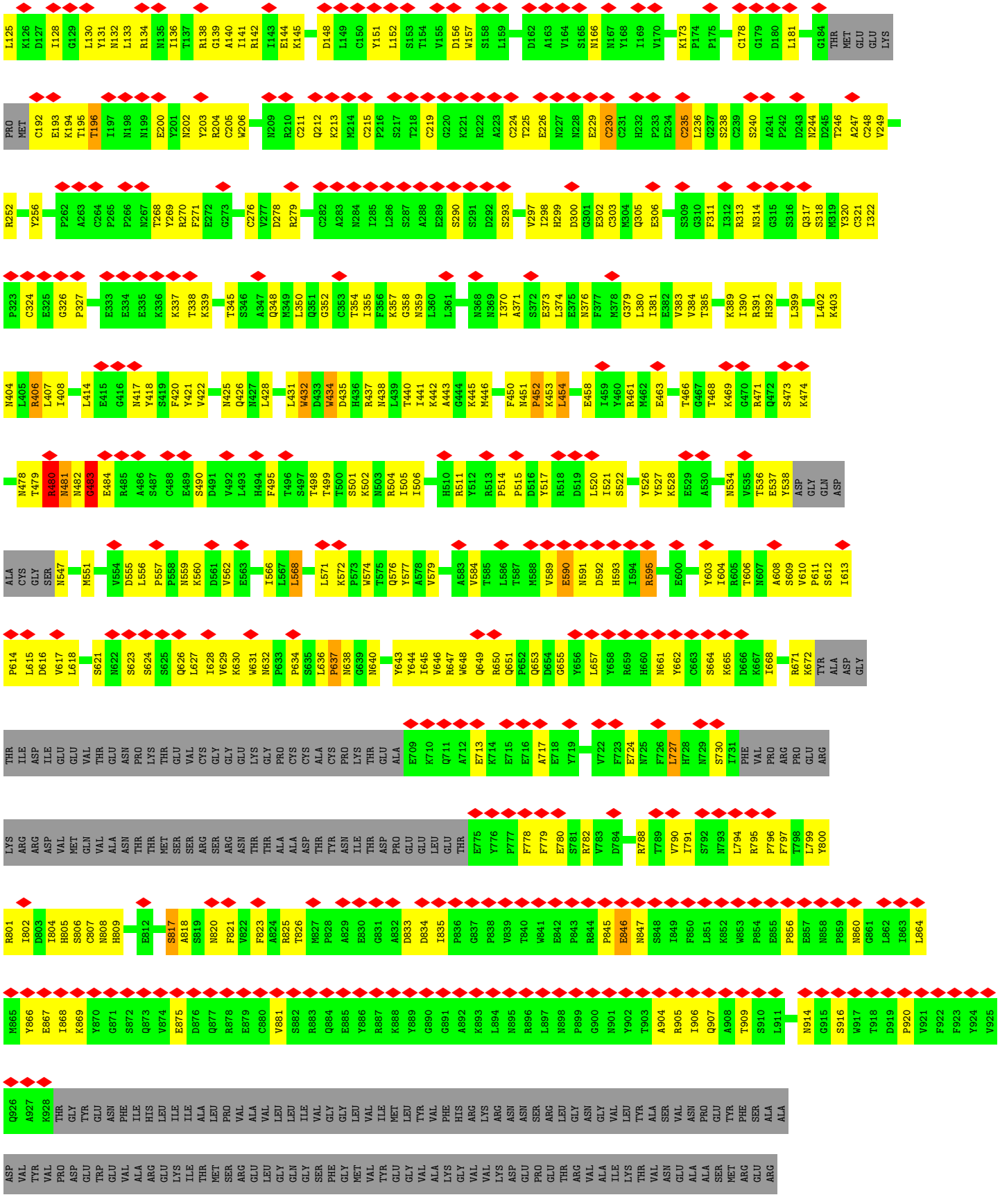


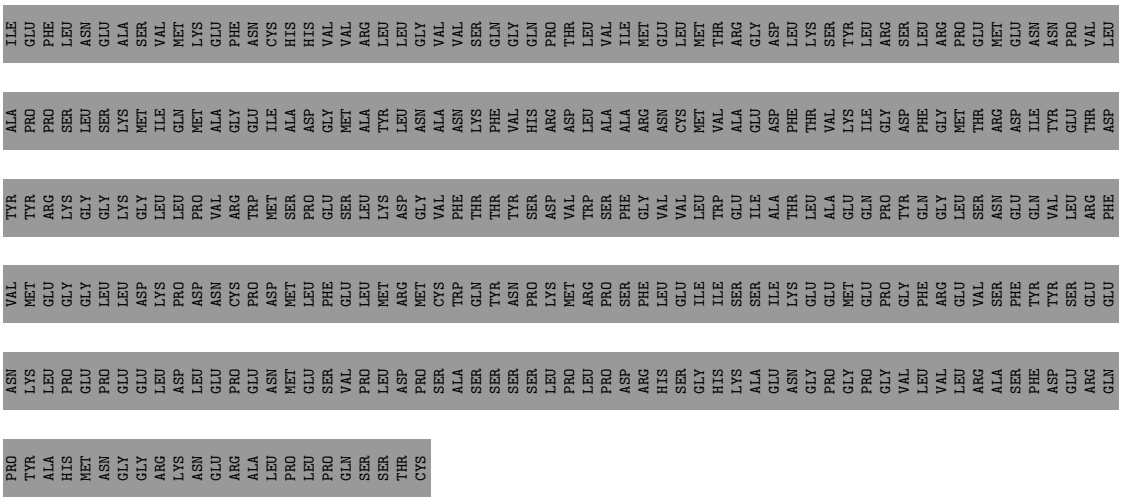
• Molecule 1: Insulin-like growth factor 1 receptor

Chain B:



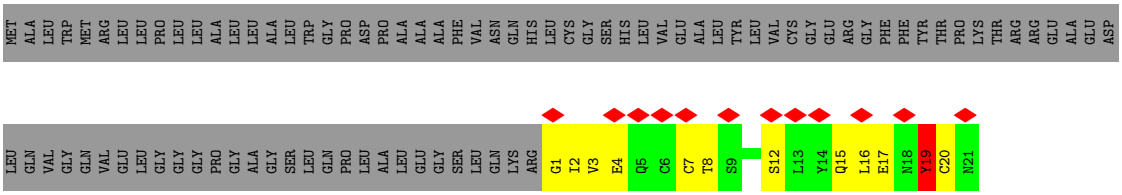



L125 K126 D127 I128 G129 L130 Y131 N132 L133 R134 N135 I136 T137 R138 G139 A140 I141 R142 I143 E144 K145 D148 L149 C150 Y151 L152 S153 T154 V155 D156 W157 S158 L159 D162 A163 V164 S165 N166 N167 Y168 I169 V170 K173 P174 P175 C178 G179 D180 L181 G184 THR MET GLU GLU LYS
PRO MET C192 E193 K194 T195 T196 I197 N198 N199 E200 Y201 N202 Y203 R204 C205 W206 N209 R210 C211 Q212 K213 N214 C215 P216 S217 T218 C219 G220 K221 R222 A223 C224 T225 E226 N227 N228 E229 C230 C231 H232 P233 E234 C235 L236 G237 S238 C239 S240 A241 P242 D243 W244 D245 T246 A247 C248 Y249
R252 Y256 P262 A263 C264 P265 P266 N267 T268 Y269 R270 F271 E272 G273 C276 V277 D278 R279 C282 A283 N284 I285 L286 S287 A288 E289 S290 S291 D292 S293 V297 I298 H299 D300 G301 E302 C303 M304 Q305 E306 S309 G310 F311 I312 R313 N314 G315 S316 Q317 S318 M319 Y320 C321 I322
P323 C324 E325 G326 P327 E333 E334 E335 K336 K337 T338 K339 T345 S346 A347 Q348 M349 L350 Q351 G352 C353 T354 I355 F356 K357 G358 N359 L360 L361 N368 N369 I370 A371 S372 E373 L374 E375 N376 F377 M378 G379 L380 I381 E382 V383 V384 T385 K389 I390 R391 H392 L399 L402 K403
N404 L405 R406 L407 I408 L414 E415 G416 N417 Y418 S419 F420 Y421 V422 N425 Q426 N427 L428 L431 W432 D433 W434 D435 H436 R437 N438 L439 T440 I441 K442 A443 G444 K445 M446 F450 N451 P452 K453 L454 E458 I459 Y460 R461 M462 E463 T466 G467 T468 K469 G470 R471 Q472 S473 K474
N478 T479 R480 N481 N482 G483 E484 R485 A486 S487 C488 E489 S490 D491 V492 L493 H494 F495 T496 S497 T498 T499 T500 S501 K502 N503 R504 I505 I506 H510 R511 Y512 R513 P514 P515 D516 Y517 R518 D519 L520 I521 S522 Y526 Y527 K528 E529 A530 N534 V535 T536 E537 Y538 ASP GLY GLN ASP
ALA CYS GLY SER N547 M551 V554 D555 L556 P557 P558 N559 K560 D561 V562 E563 I566 L567 L568 L571 K572 P573 W574 T575 Q576 Y577 A578 V579 A583 V584 T585 L586 T587 M588 V589 E590 N591 D592 H593 I594 R595 E600 Y603 I604 R605 T606 N607 A608 S609 V610 P611 S612 I613
P614 L615 D616 V617 L618 S621 M622 S623 S624 S625 Q626 L627 I628 V629 K630 W631 N632 P633 P634 S635 L636 P637 N638 G639 N640 Y643 Y644 I645 V646 R647 W648 Q649 R650 Q651 P652 Q653 D654 G655 Y656 L657 Y658 R659 H660 N661 Y662 C663 S664 K665 D666 K667 I668 R671 K672 TYR ALA ASP GLY
THR ILE ASP ILE GLU GLU VAL THR GLU ASN PRO LYS THR GLU VAL CYS GLY GLY GLU LYS GLY PRO CYS CYS ALA CYS PRO LYS THR GLU ALA E709 K710 Q711 A712 E713 K714 E715 E716 A717 E718 Y719 V722 F723 E724 N725 F726 L727 H728 N729 S730 I731 PHE VAL PRO ARG PRO GLU ARG
LYS ARG ARG ASP VAL MET GLN VAL ALA ASN THR THR MET SER SER ARG SER ARG ASN THR THR ALA ALA ASP THR TYR ASN ILE THR ASP PRO GLU GLU LEU GLU THR E775 Y776 P777 F778 F779 E780 S781 R782 V783 D784 R788 T789 V790 I791 S792 N793 L794 R795 P796 F797 T798 L799 Y800
R801 I802 D803 I804 H805 S806 C807 N808 H809 E812 S817 A818 S819 N820 F821 V822 F823 A824 R825 T826 W827 P828 A829 E830 G831 A832 D833 D834 I835 P836 G837 P838 V839 T840 W841 E842 P843 R844 P845 E846 N847 S848 I849 F850 L851 K852 W853 P854 E855 P856 E857 N858 P859 N860 G861 L862 I863 L864
M865 Y866 E867 I868 K869 Y870 G871 S872 Q873 V874 E875 D876 Q877 R878 E879 C880 V881 S882 R883 Q884 E885 Y886 R887 K888 Y889 G890 G891 A892 K893 L894 N895 R896 L897 N898 P899 G900 N901 Y902 T903 A904 R905 I906 Q907 A908 T909 S910 L911 N914 G915 S916 W917 T918 D919 P920 V921 F922 F923 Y924 V925
Q926 A927 K928 THR GLY TYR GLU ASN PHE ILE HIS LEU ILE ILE ALA LEU PRO VAL ALA VAL LEU LEU ILE VAL GLY GLY LEU VAL ILE MET LEU TYR VAL PHE HIS ARG LYS ARG ASN ASN SER ARG LEU GLY ASN GLY VAL LEU TYR THR ALA SER VAL ASN PRO GLU TYR PHE SER ALA ALA
ASP VAL TYR VAL PRO ASP GLU TRP GLU VAL ALA ARG GLU LYS ILE THR MET SER ARG GLU LEU GLY GLN GLY SER PHE GLY MET VAL TYR GLU GLY VAL ALA LYS GLY VAL VAL LYS ASP GLU PRO GLU THR ARG VAL ALA ILE LYS THR VAL ASN GLU GLU ALA ALA SER MET ARG GLU ARG



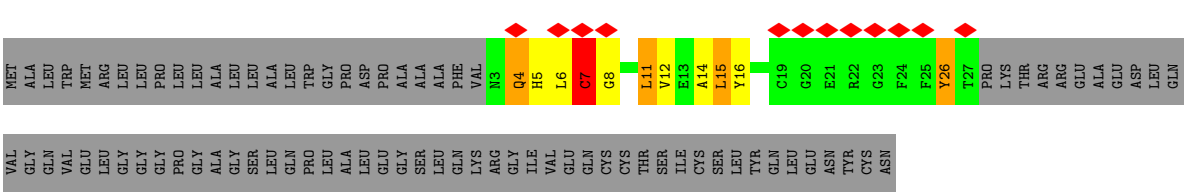
• Molecule 2: Insulin

Chain C:



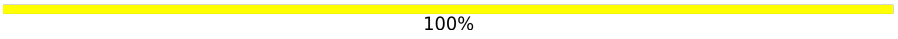
• Molecule 2: Insulin

Chain D:



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

Chain E:



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

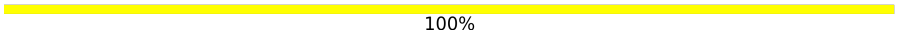
Chain G:

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

Chain H:

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

Chain I:



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

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	36496	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	219.2, 219.2, 219.2	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.49	3/6753 (0.0%)	0.92	21/9161 (0.2%)
1	B	0.46	0/6604	0.89	19/8951 (0.2%)
2	C	0.82	1/164 (0.6%)	1.19	0/220
2	D	0.90	1/218 (0.5%)	1.74	6/294 (2.0%)
All	All	0.49	5/13739 (0.0%)	0.93	46/18626 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	24
2	D	0	1
All	All	0	42

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	CYS	CA-CB	6.68	1.68	1.53
1	A	866	TYR	CD2-CE2	-6.11	1.30	1.39
2	C	19	TYR	CD2-CE2	-5.17	1.31	1.39
1	A	549	TRP	CB-CG	-5.03	1.41	1.50
1	A	387	TYR	CD2-CE2	-5.01	1.31	1.39

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	CYS	CA-CB-SG	11.93	135.47	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	15	LEU	CB-CG-CD2	-11.74	91.05	111.00
1	B	219	CYS	CA-CB-SG	-9.21	97.41	114.00
1	A	52	CYS	CA-CB-SG	8.31	128.95	114.00
1	B	235	CYS	CA-CB-SG	8.08	128.54	114.00

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASP	Peptide
1	A	227	ASN	Peptide
1	A	368	ASN	Peptide
1	A	393	SER	Peptide
1	A	62	LEU	Peptide

5.2 Too-close contacts (i)

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	6595	0	6377	251	0
1	B	6450	0	6268	229	0
2	C	163	0	149	11	0
2	D	212	0	192	10	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	F	50	0	43	3	0
5	A	42	0	39	0	0
5	B	42	0	39	2	0
All	All	13666	0	13207	486	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 18.

The worst 5 of 486 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:802:ILE:O	1:B:821:PHE:HA	1.55	1.04
1:A:492:VAL:HA	1:A:598:LYS:O	1.57	1.02
1:B:609:SER:O	1:B:808:ASN:ND2	1.96	0.99
1:B:640:ASN:HD21	5:B:1407:NAG:C1	1.74	0.99
1:A:904:ALA:O	1:A:920:PRO:HA	1.63	0.98

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	811/1367 (59%)	687 (85%)	121 (15%)	3 (0%)	30 68
1	B	790/1367 (58%)	682 (86%)	98 (12%)	10 (1%)	10 42
2	C	19/110 (17%)	15 (79%)	4 (21%)	0	100 100
2	D	24/110 (22%)	18 (75%)	6 (25%)	0	100 100
All	All	1644/2954 (56%)	1402 (85%)	229 (14%)	13 (1%)	19 54

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	846	GLU
1	A	876	ASP
1	B	83	GLU
1	B	481	ASN
1	B	592	ASP

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	734/1204 (61%)	709 (97%)	25 (3%)	32 52
1	B	718/1204 (60%)	713 (99%)	5 (1%)	81 87
2	C	20/88 (23%)	19 (95%)	1 (5%)	20 42
2	D	22/88 (25%)	22 (100%)	0	100 100
All	All	1494/2584 (58%)	1463 (98%)	31 (2%)	49 67

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	LEU
1	B	324	CYS
1	A	502	LYS
1	B	480	ARG
1	A	905	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	640	ASN
2	D	4	GLN
2	C	15	GLN
1	B	284	ASN
1	B	632	ASN

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)

12 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	E	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	1.01	1 (5%)
3	NAG	E	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.20	3 (17%)
4	NAG	F	1	1,4	14,14,15	1.39	1 (7%)	17,19,21	0.76	0
4	NAG	F	2	4	14,14,15	0.51	0	17,19,21	0.61	0
4	MAN	F	3	4	11,11,12	1.80	1 (9%)	15,15,17	1.30	2 (13%)
4	MAN	F	4	4	11,11,12	0.89	0	15,15,17	1.10	2 (13%)
3	NAG	G	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	H	1	3,1	14,14,15	0.58	0	17,19,21	0.58	0
3	NAG	H	2	3	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
3	NAG	I	1	3,1	14,14,15	1.06	1 (7%)	17,19,21	1.06	1 (5%)
3	NAG	I	2	3	14,14,15	0.43	0	17,19,21	0.61	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	MAN	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	MAN	C1-C2	5.69	1.65	1.52
4	F	1	NAG	O5-C1	-4.99	1.35	1.43
3	E	2	NAG	C1-C2	4.57	1.59	1.52
3	I	1	NAG	O5-C1	-3.68	1.37	1.43
3	E	1	NAG	O5-C1	-2.77	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C4-C3-C2	2.92	115.29	111.02
4	F	3	MAN	C1-O5-C5	2.85	116.05	112.19
3	E	2	NAG	C1-O5-C5	2.67	115.81	112.19
3	I	1	NAG	O4-C4-C3	-2.60	104.34	110.35
3	E	2	NAG	O5-C5-C4	-2.57	104.58	110.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

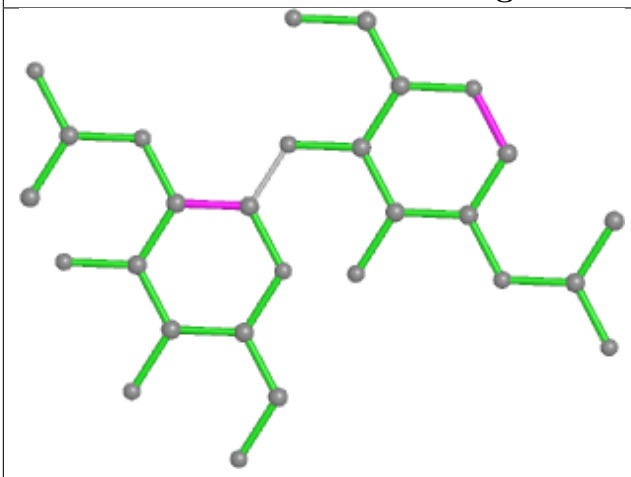
There are no ring outliers.

4 monomers are involved in 3 short contacts:

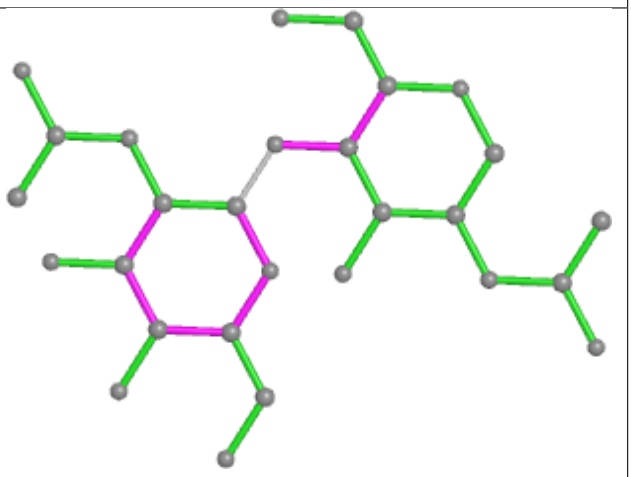
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	F	4	MAN	1	0
4	F	3	MAN	1	0
4	F	1	NAG	1	0

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

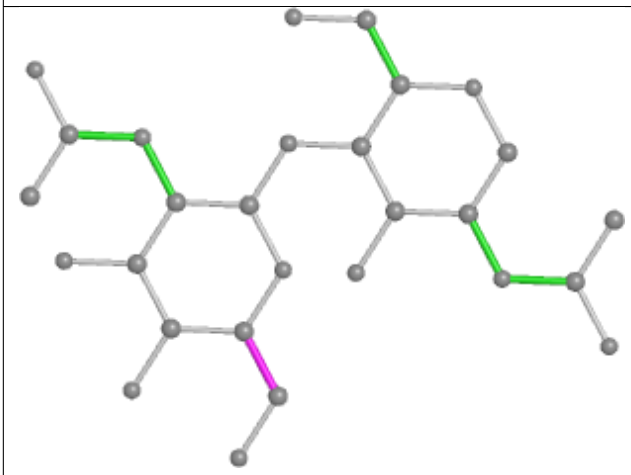
Oligosaccharide Chain E



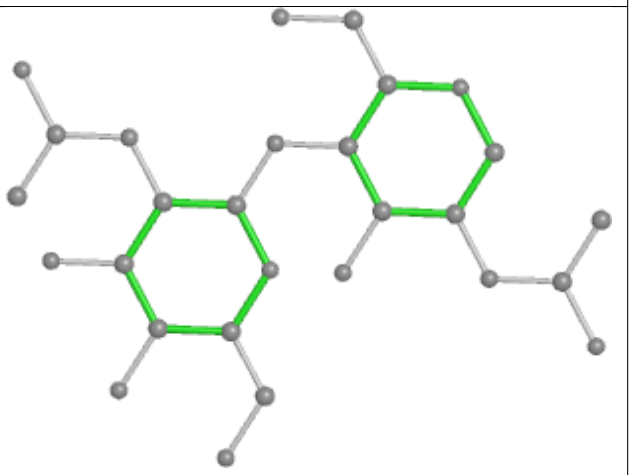
Bond lengths



Bond angles

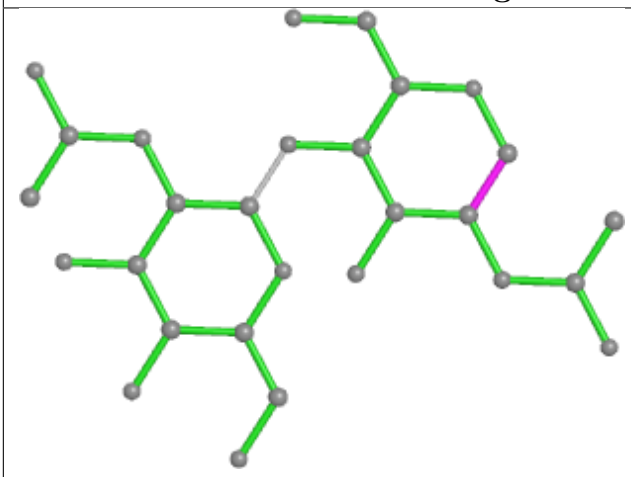


Torsions

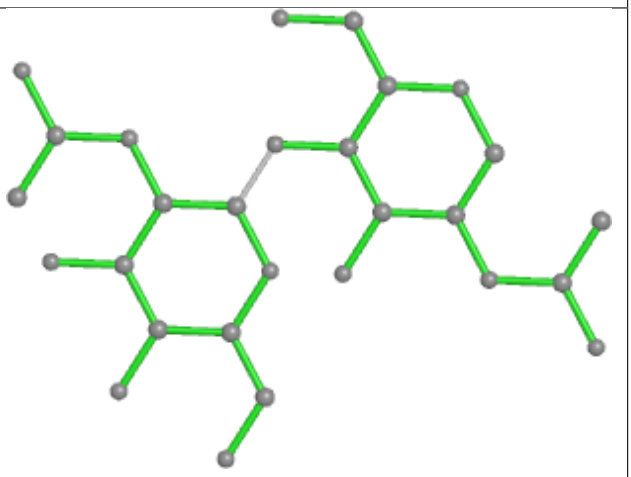


Rings

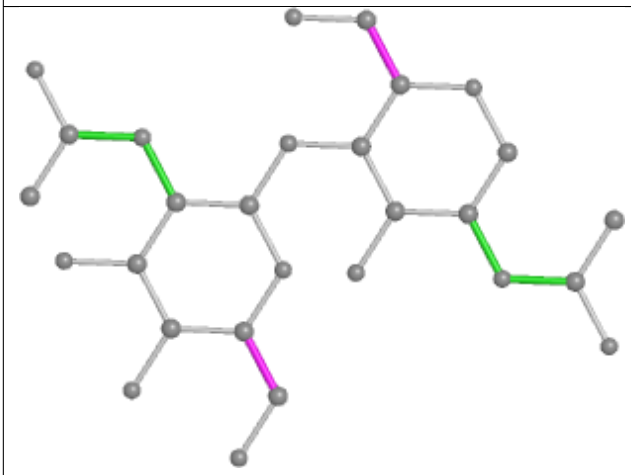
Oligosaccharide Chain G



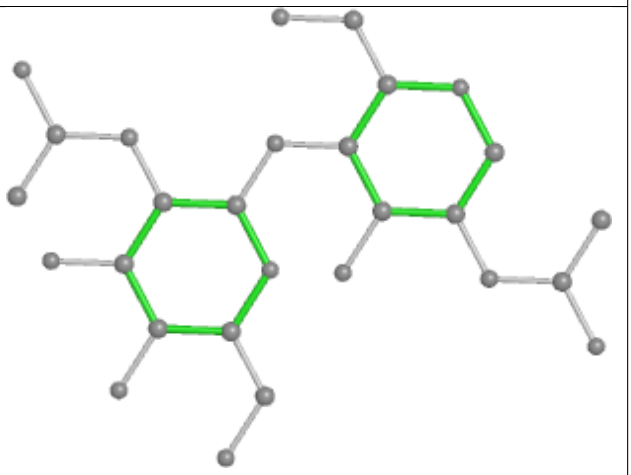
Bond lengths



Bond angles

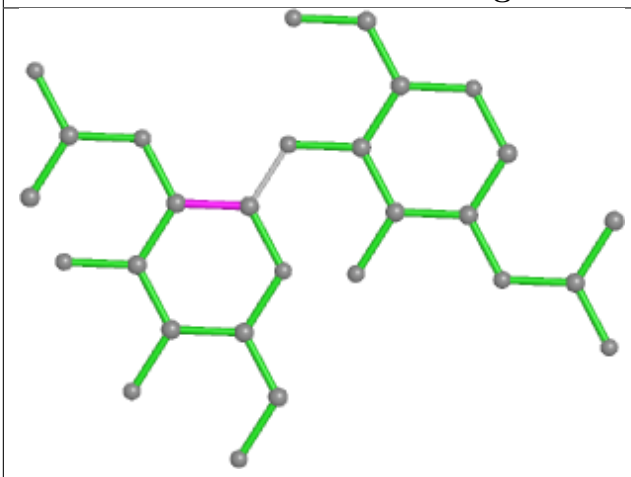


Torsions

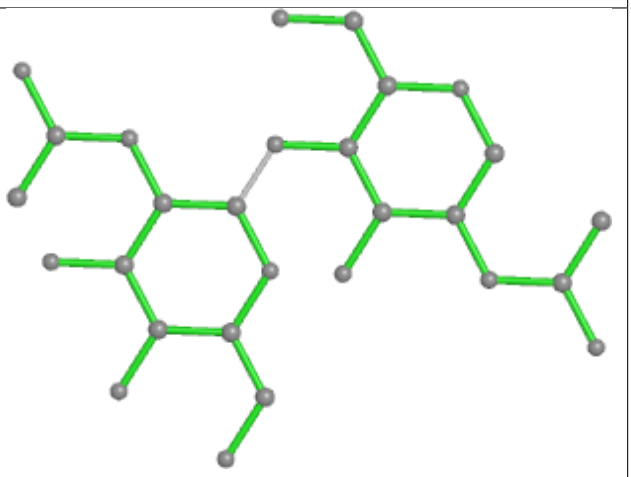


Rings

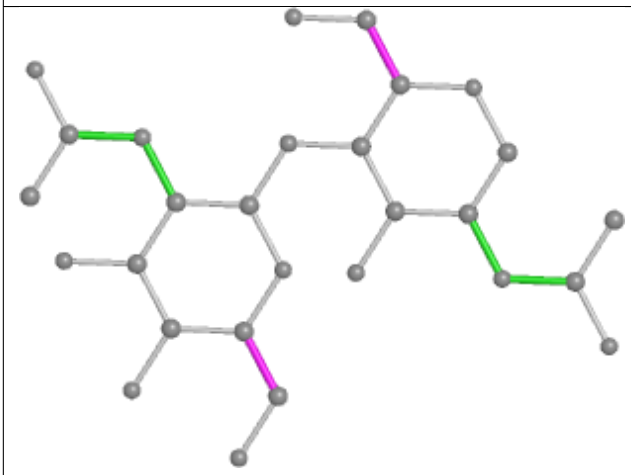
Oligosaccharide Chain H



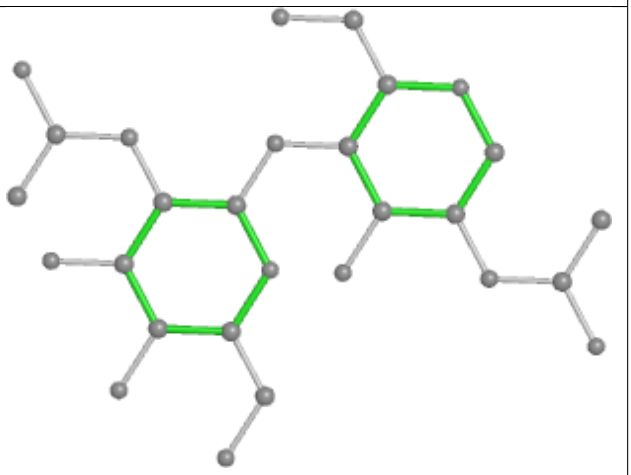
Bond lengths



Bond angles

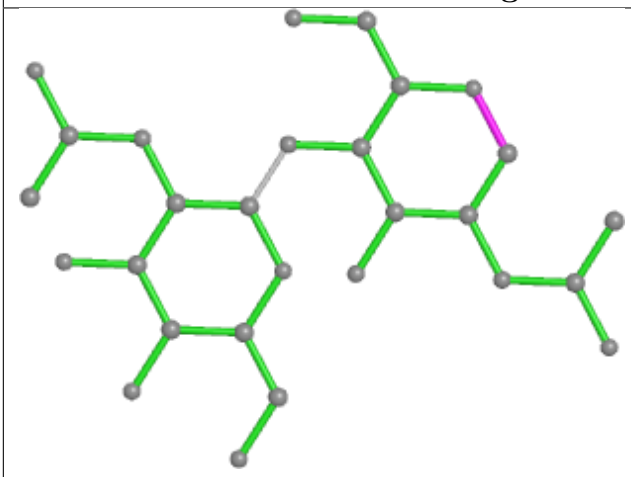


Torsions

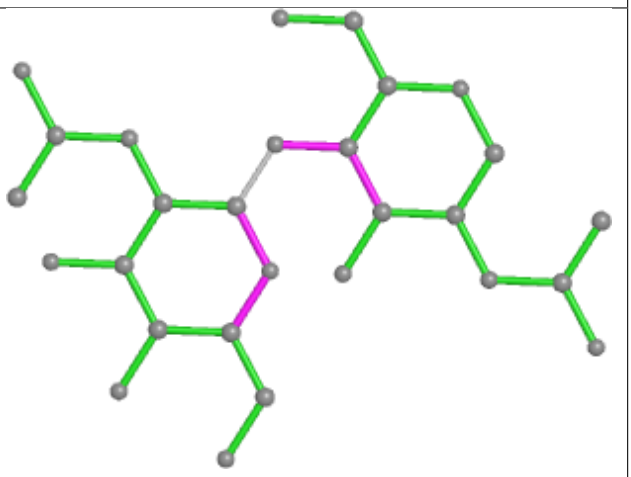


Rings

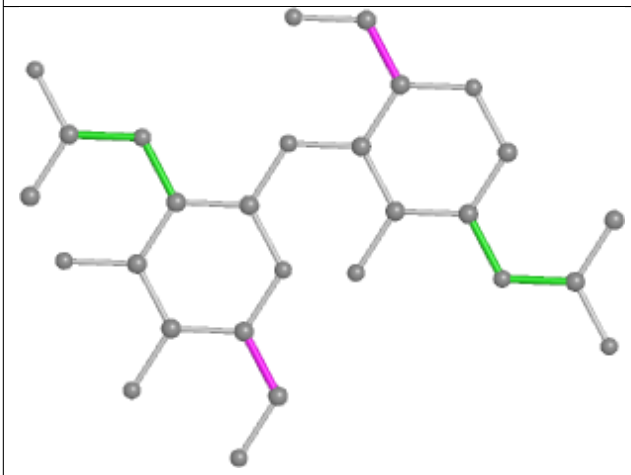
Oligosaccharide Chain I



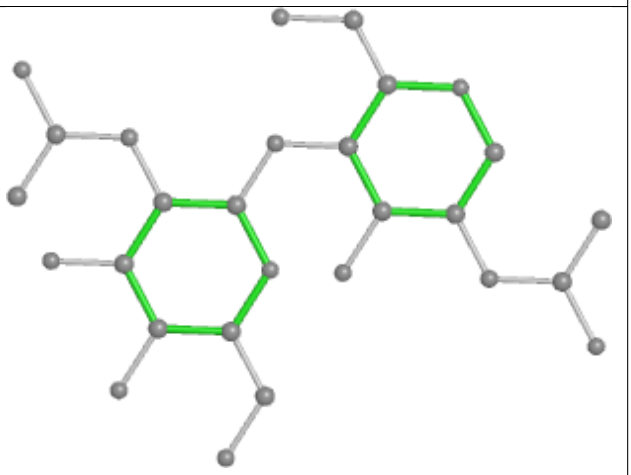
Bond lengths



Bond angles

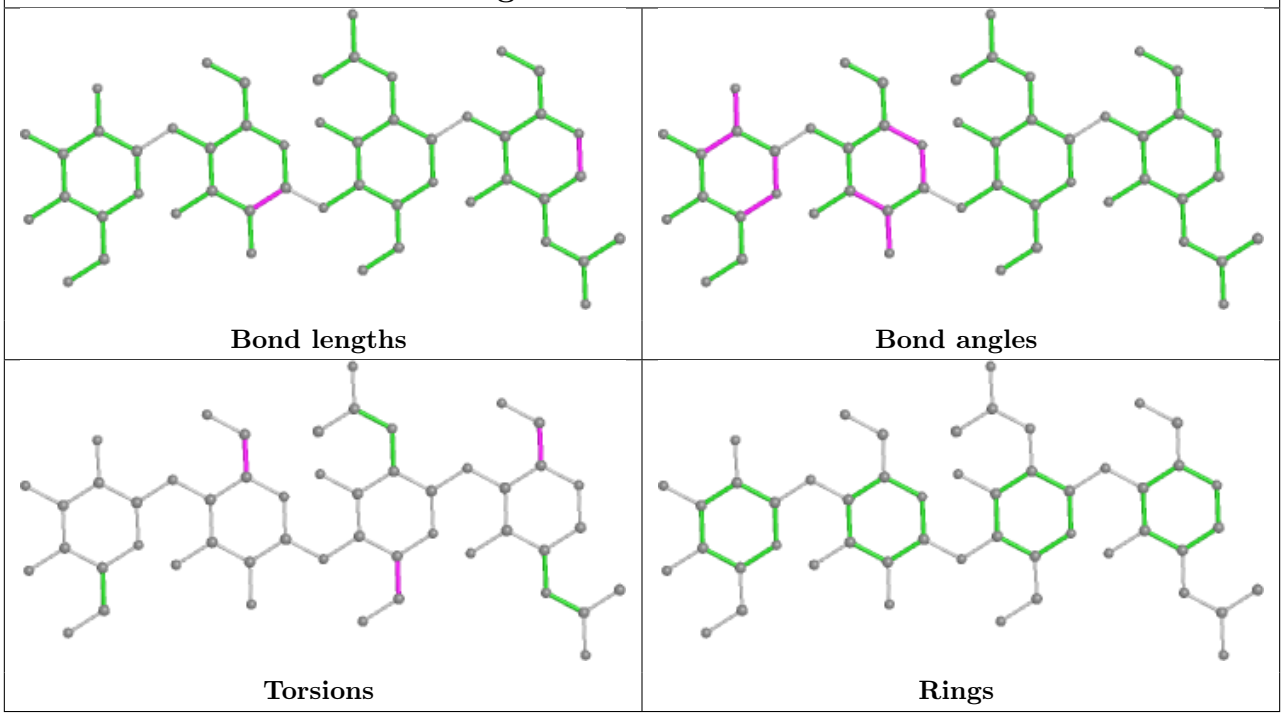


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

6 ligands 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	$\#\|Z\| > 2$
5	NAG	A	1401	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
5	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
5	NAG	B	1401	1	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
5	NAG	A	1404	1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
5	NAG	B	1404	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	B	1407	-	14,14,15	0.42	0	17,19,21	0.71	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1409	NAG	C2-N2-C7	3.13	127.36	122.90
5	B	1401	NAG	C2-N2-C7	3.11	127.33	122.90
5	A	1401	NAG	C2-N2-C7	3.04	127.23	122.90
5	B	1407	NAG	C1-O5-C5	2.46	115.53	112.19
5	B	1404	NAG	C1-O5-C5	2.29	115.29	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1404	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1409	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1407	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

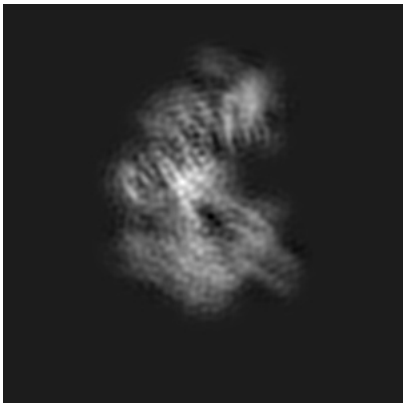
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9838. These allow visual inspection of the internal detail of the map and identification of artifacts.

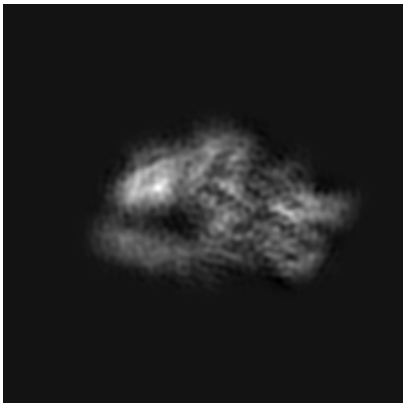
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

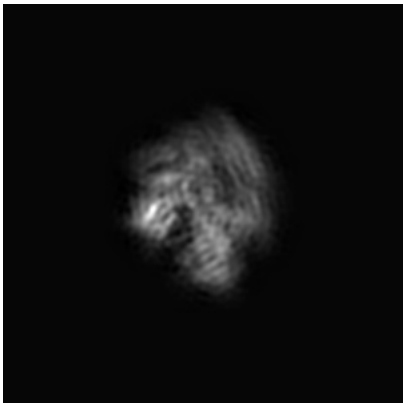
6.1.1 Primary map



X



Y

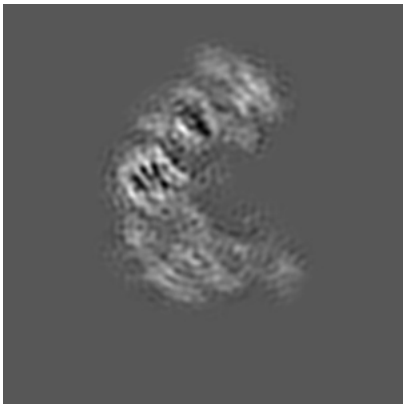


Z

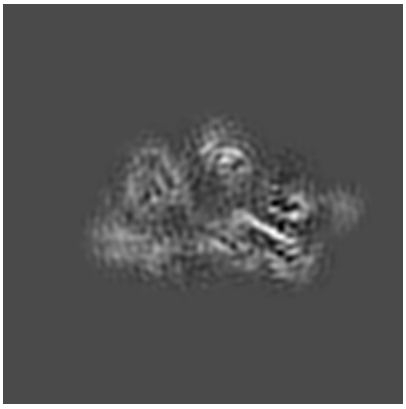
The images above show the map projected in three orthogonal directions.

6.2 Central slices

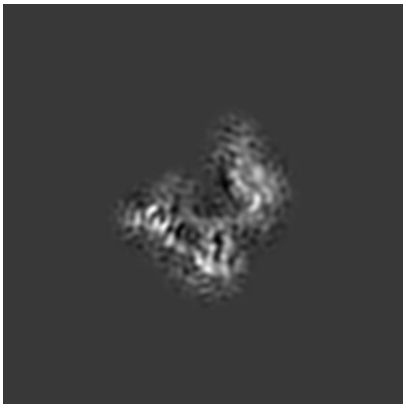
6.2.1 Primary map



X Index: 80



Y Index: 80

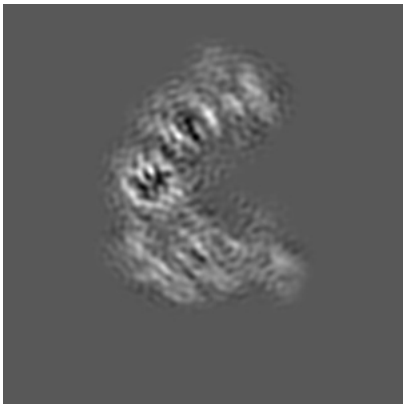


Z Index: 80

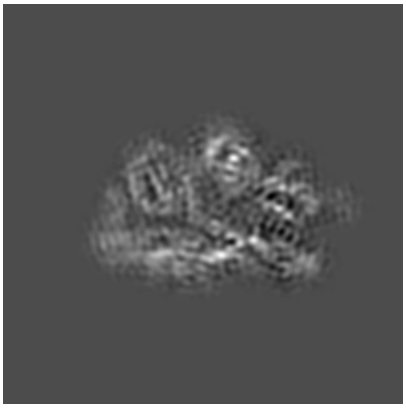
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 82



Y Index: 76

Z Index: 90

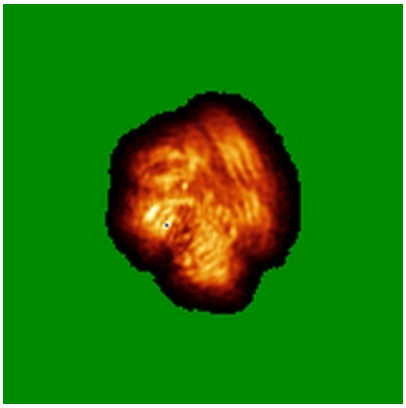
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

X

Y



Z

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 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

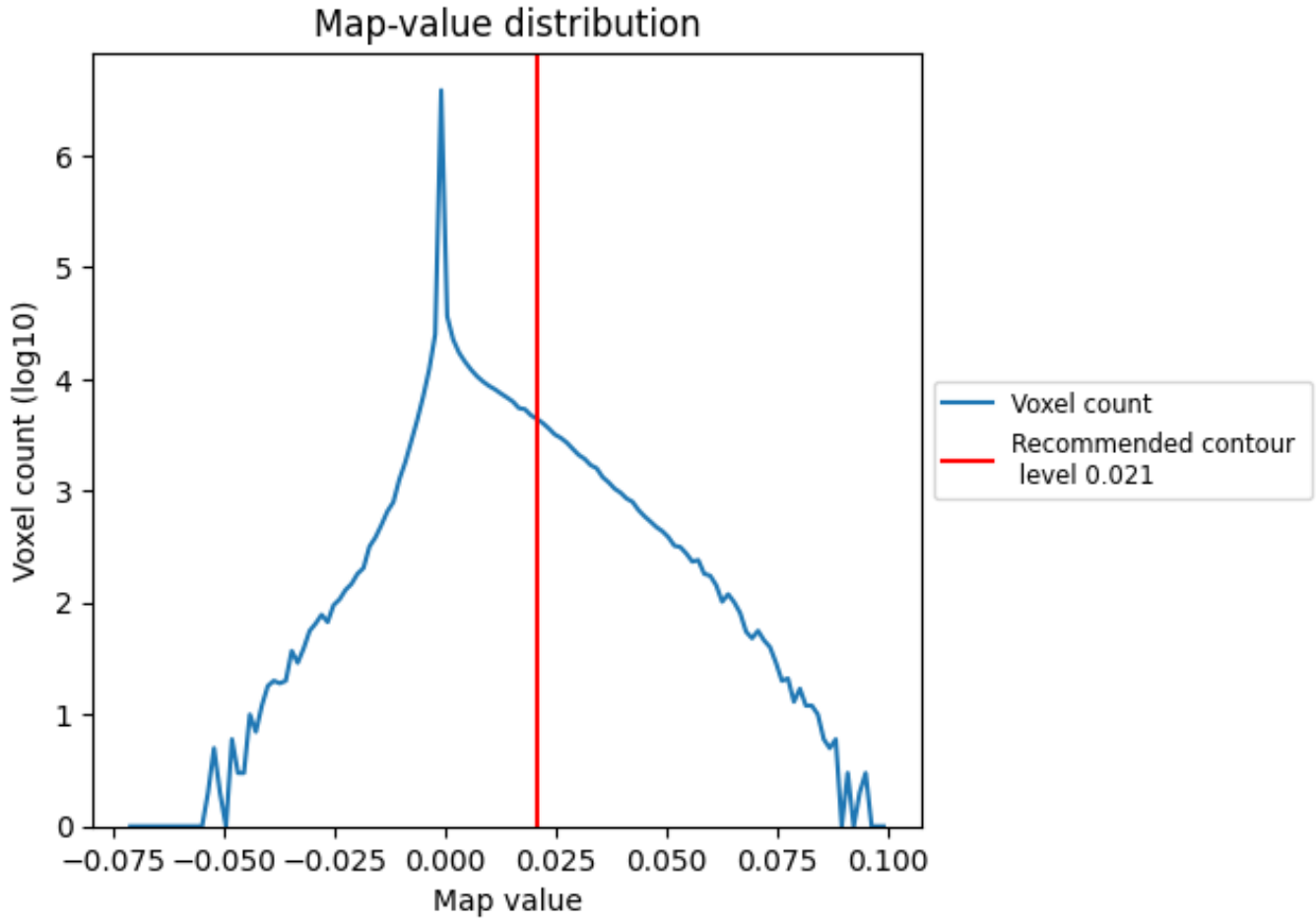
6.6 Mask visualisation (i)

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

7 Map analysis

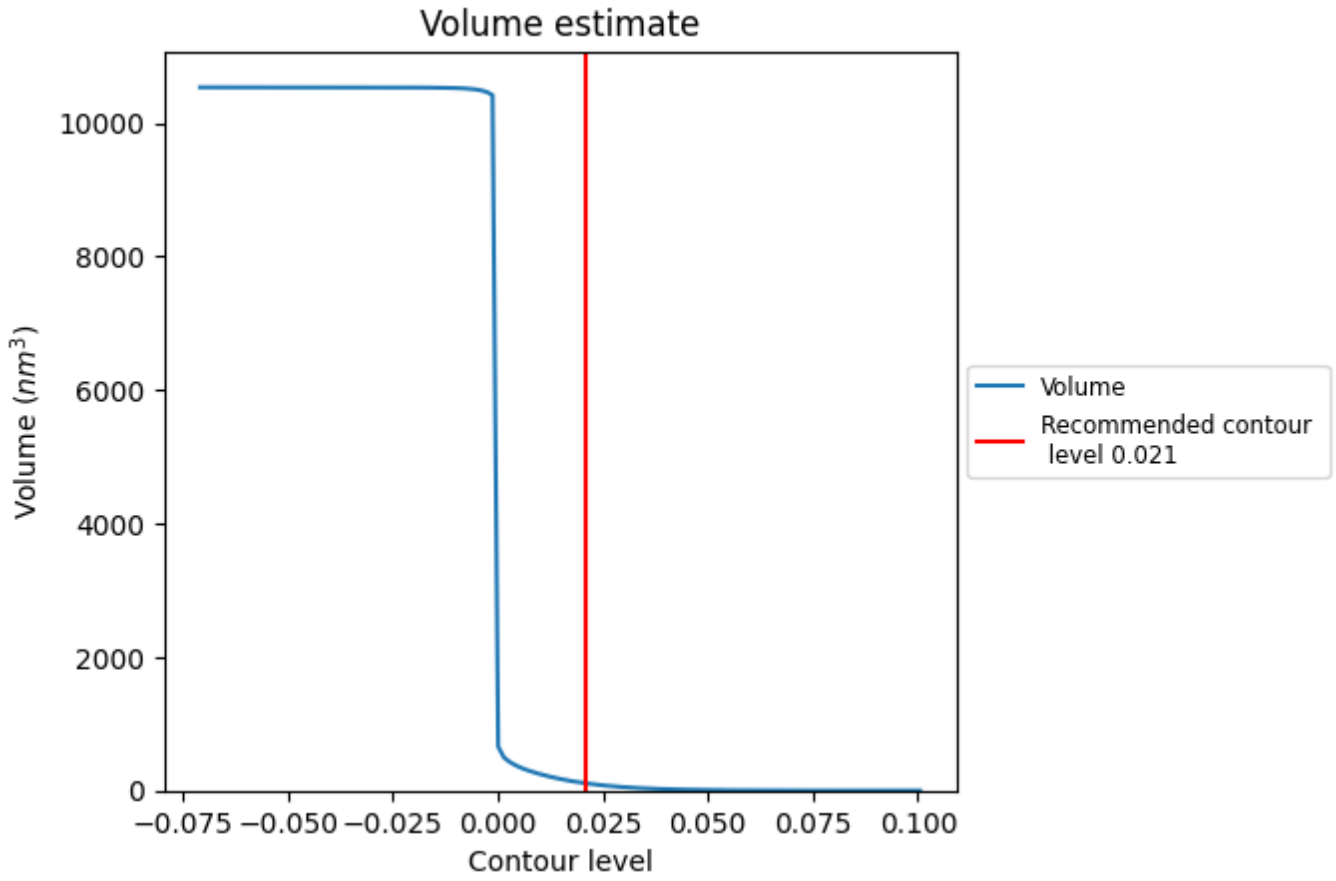
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

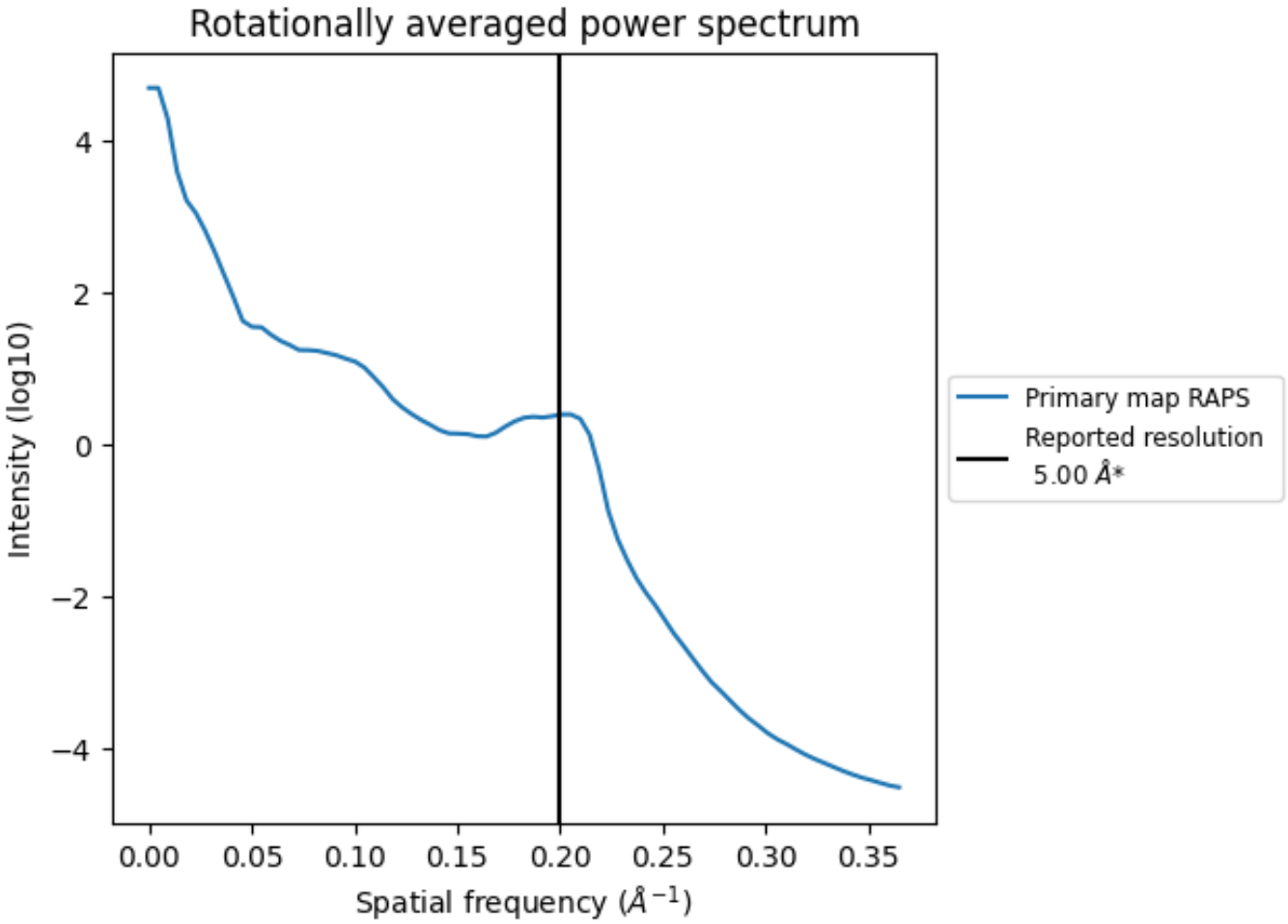
7.2 Volume estimate (i)



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 98 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)

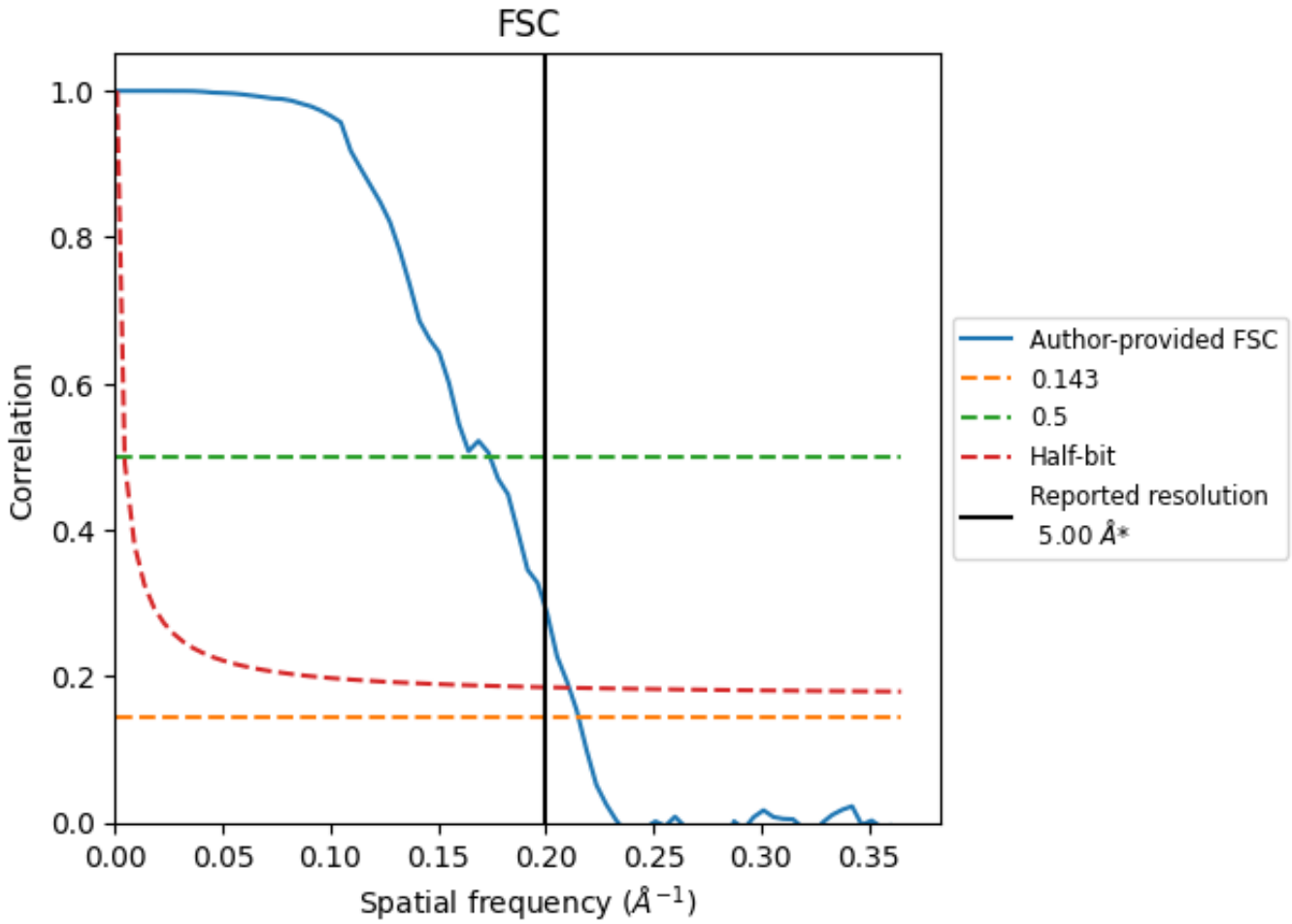


*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

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 0.200 Å^{-1}

8.2 Resolution estimates (i)

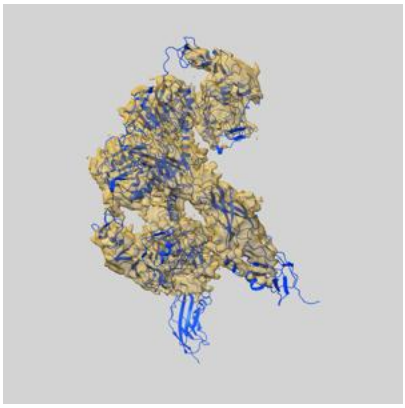
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.65	5.74	4.74
Unmasked-calculated*	-	-	-

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

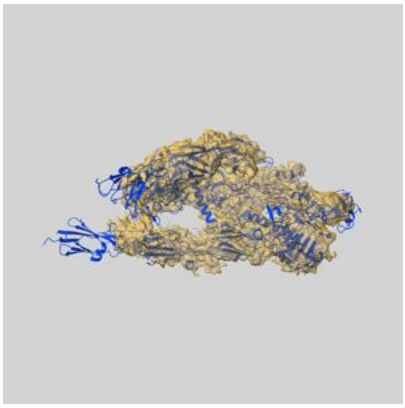
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9838 and PDB model 6JK8. Per-residue inclusion information can be found in section 3 on page 6.

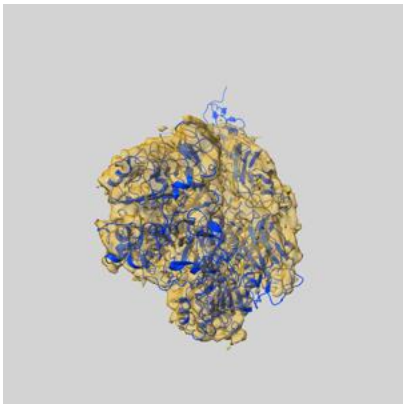
9.1 Map-model overlay



X



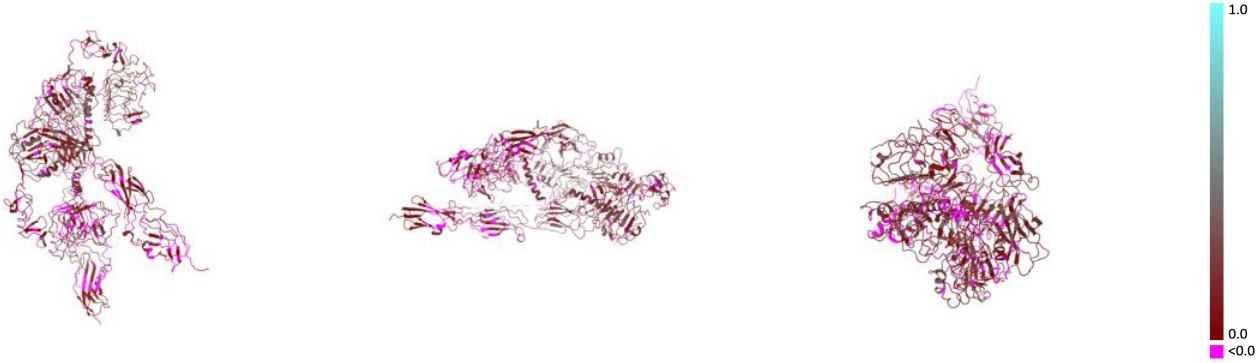
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

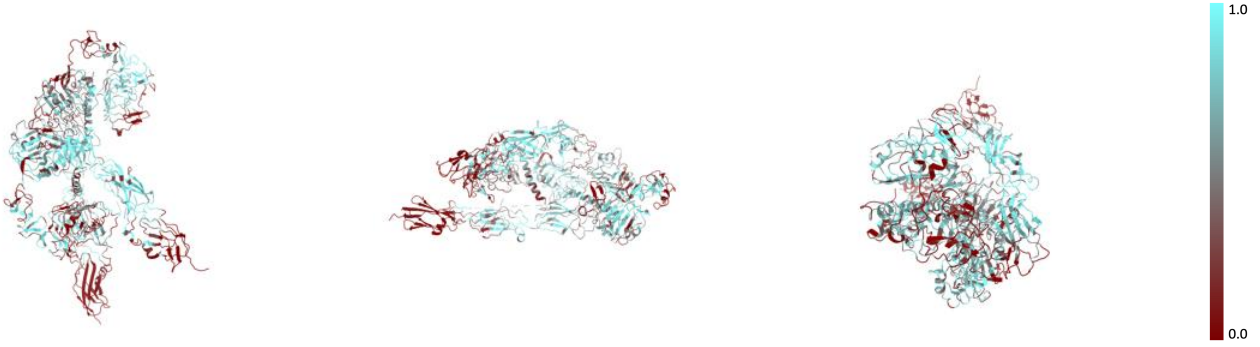
9.2 Q-score mapped to coordinate model (i)



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.

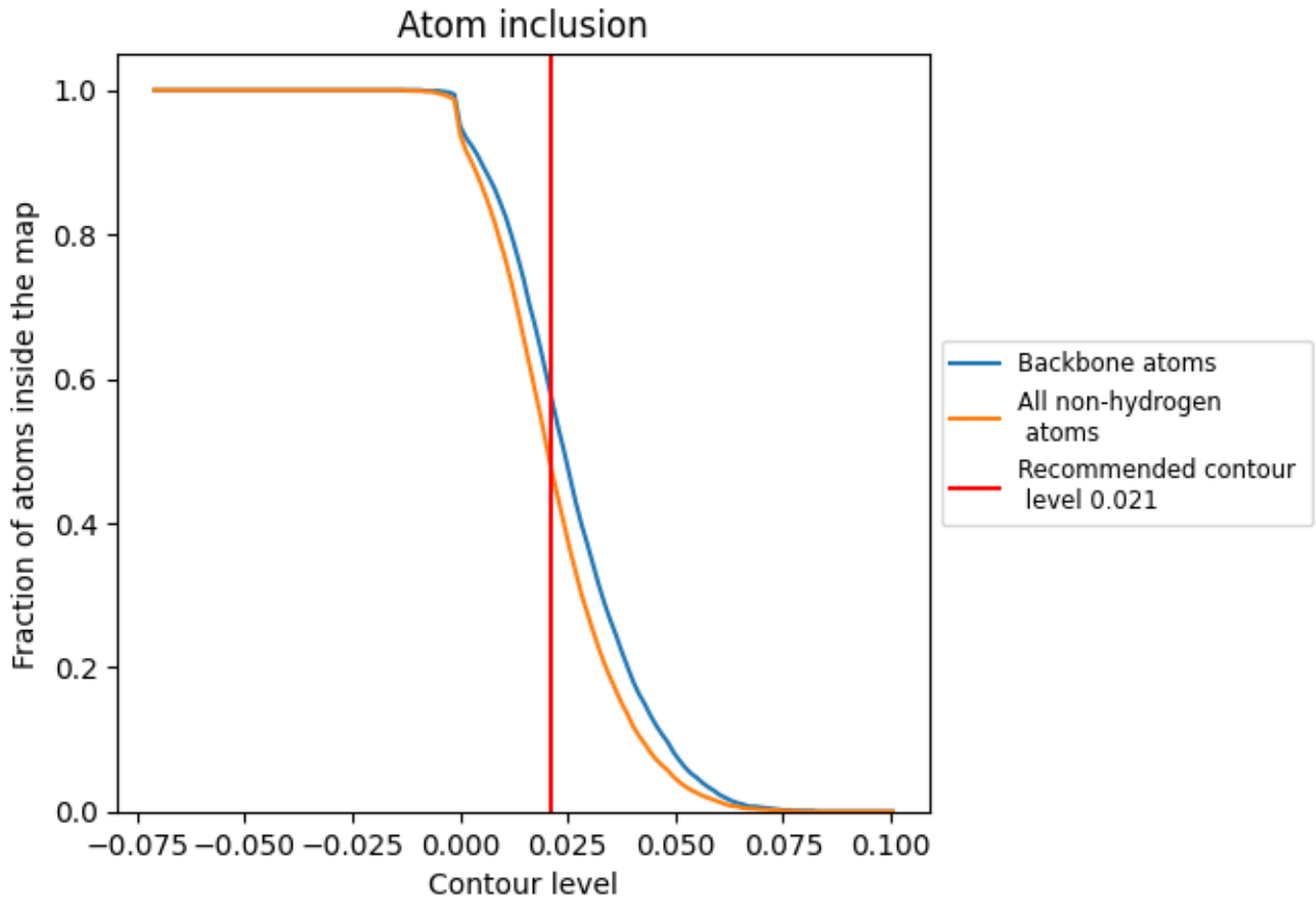
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4800	0.1220
A	0.5070	0.1330
B	0.4570	0.1100
C	0.3730	0.1010
D	0.4340	0.1620
E	0.9290	0.3520
F	0.3000	0.1020
G	0.2140	-0.0360
H	0.4290	0.1470
I	0.7500	0.2880