wwPDB EM Validation Summary Report (i)

Nov 6, 2022 – 09:01 PM EST

PDB ID	:	6NJM
EMDB ID	:	EMD-9388
Title	:	Architecture and subunit arrangement of native AMPA receptors
Authors	:	Gouaux, E.; Zhao, Y.
Deposited on	:	2019-01-03
Resolution	:	6.50 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

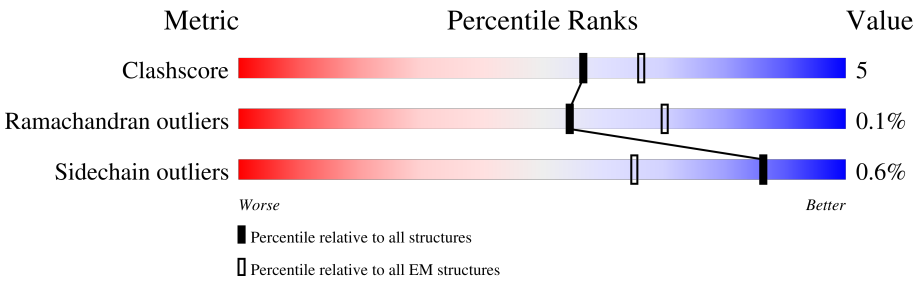
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.50 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	888	45% 78% 9% • 12%
1	C	888	48% 78% 10% • 12%
2	B	883	47% 82% 6% 11%
2	D	883	50% 82% 7% 11%
3	E	153	50% 76% 24%
3	G	153	43% 76% 24%
4	F	323	26% 52% • 48%
4	H	323	29% 52% • 48%

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Mol	Chain	Length	Quality of chain
5	I	218	68% 86% 14%
5	M	218	56% 87% 13%
6	J	247	30% 75% 11% 14%
6	N	247	30% 75% 11% 14%
7	K	225	45% 92% • 6%
7	O	225	34% 92% • 6%
8	L	262	56% 77% 5% 18%
8	P	262	55% 77% 5% 18%
9	Q	3	100% 33% 67%
9	S	3	100% 33% 67%
9	T	3	100% 67% 33%
9	V	3	100% 33% 33% 33%
10	R	2	100% 50% 50%
10	U	2	50% 50% 50%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 35458 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 Glutamate receptor 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	784	6011	3866	995	1116	34	0	0
1	C	784	6011	3866	995	1116	34	0	0

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	783	5684	3664	903	1091	26	0	0
2	D	783	5680	3661	902	1091	26	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
B	744	ALA	THR	conflict	UNP P19491
B	745	ALA	PRO	conflict	UNP P19491
B	754	ALA	SER	conflict	UNP P19491
B	758	ALA	VAL	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	744	ALA	THR	conflict	UNP P19491
D	745	ALA	PRO	conflict	UNP P19491
D	754	ALA	SER	conflict	UNP P19491
D	758	ALA	VAL	conflict	UNP P19491

- Molecule 3 is a protein called A'-C' auxiliary proteins.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	117	585	351	117	117	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	117	585	351	117	117	0	0

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	169	1007	645	173	186	3	0	0
4	H	169	1007	645	173	186	3	0	0

- Molecule 5 is a protein called 5B2 Fab Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	I	218	1090	654	218	218	0	0
5	M	218	1090	654	218	218	0	0

- Molecule 6 is a protein called 5B2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	213	1065	639	213	213	0	0
6	N	213	1065	639	213	213	0	0

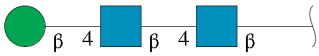
- Molecule 7 is a protein called 15F1 Fab light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	K	211	1042	620	211	211	0	0
7	O	211	1042	620	211	211	0	0

- Molecule 8 is a protein called 15F1 Fab heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	L	215	1059	629	215	215	0	0
8	P	215	1059	629	215	215	0	0

- Molecule 9 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.

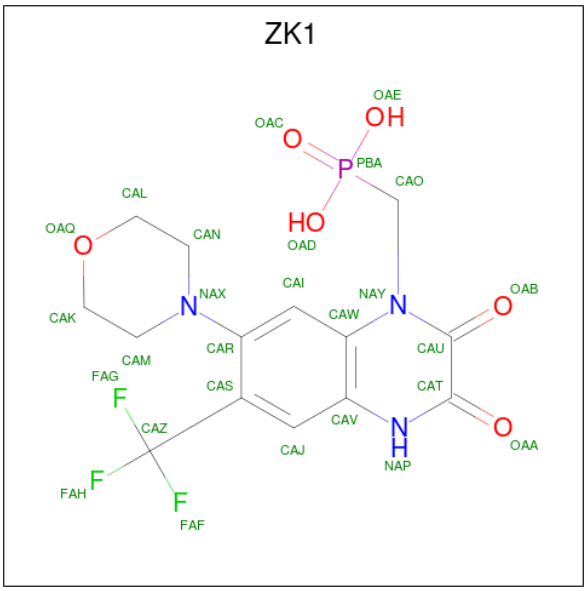


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Q	3	39	22	2	15	0	0
9	S	3	39	22	2	15	0	0
9	T	3	39	22	2	15	0	0
9	V	3	39	22	2	15	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

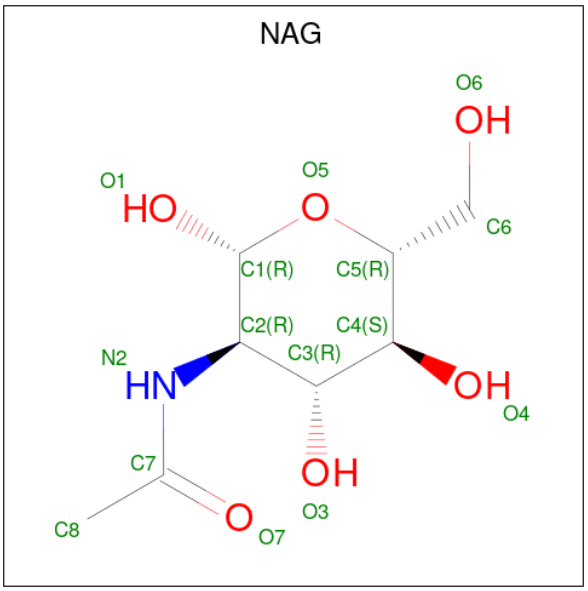
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	R	2	28	16	2	10	0	0
10	U	2	28	16	2	10	0	0

- Molecule 11 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	P	
11	A	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
11	B	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
11	C	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
11	D	1	27	14	3	3	6	1	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



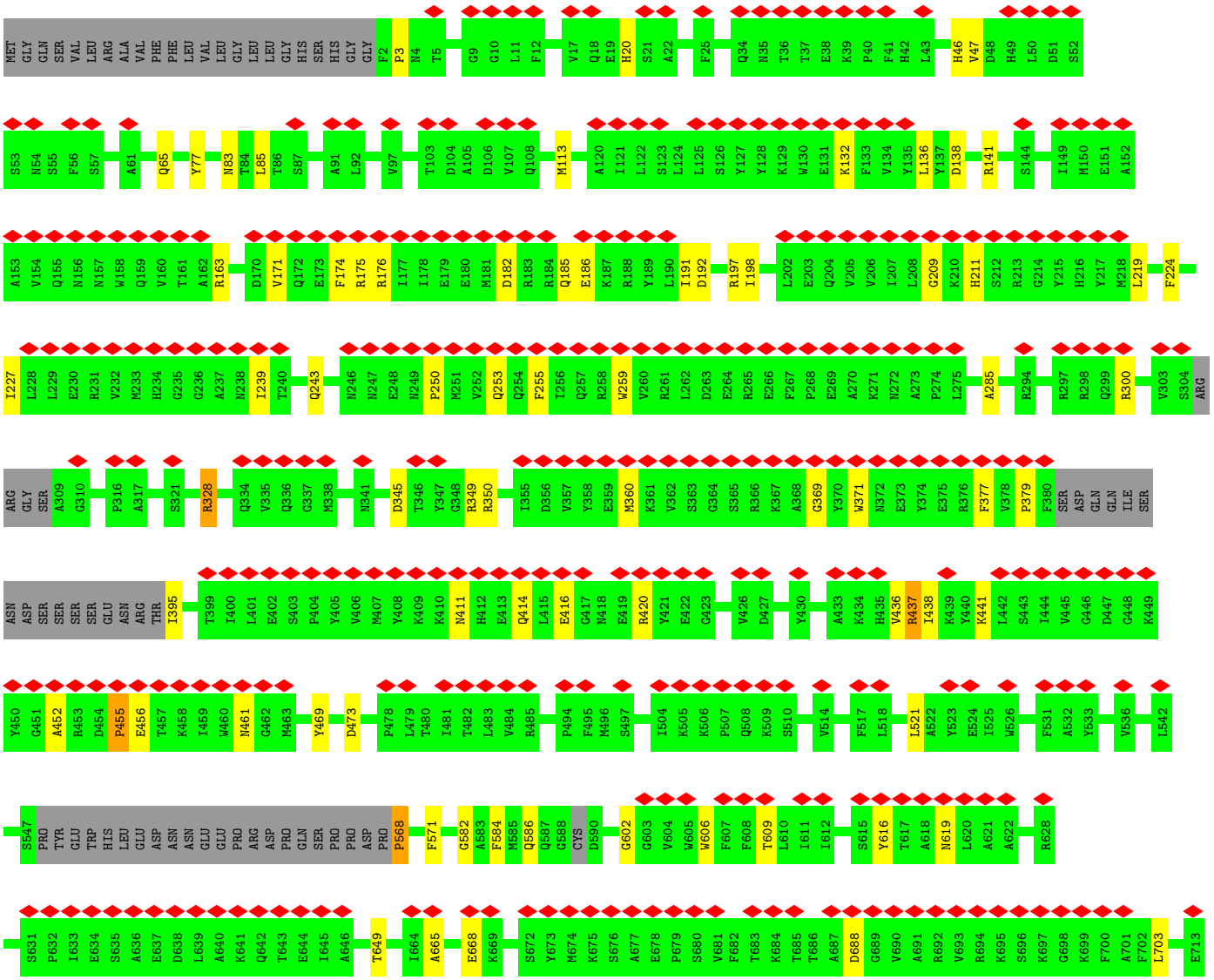
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	A	1	14	8	1	5	0
12	B	1	14	8	1	5	0
12	C	1	14	8	1	5	0
12	D	1	14	8	1	5	0

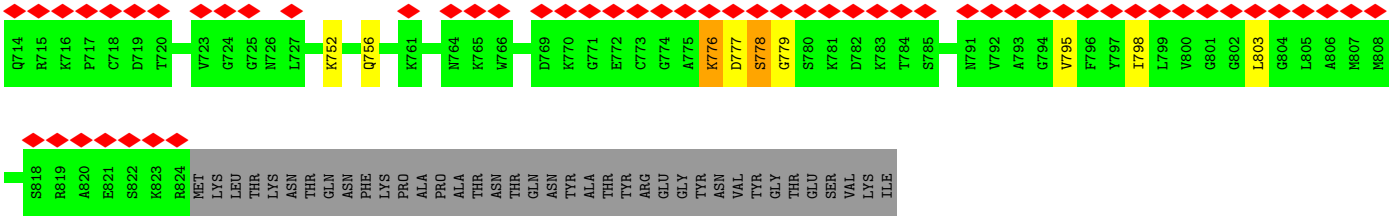
3 Residue-property plots (i)

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: Glutamate receptor 3

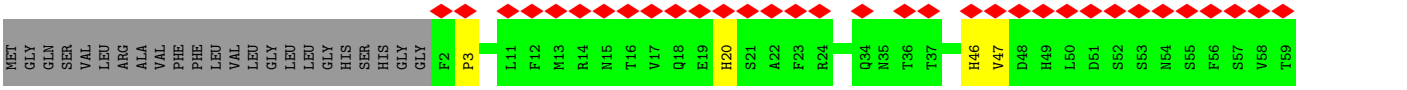
Chain A:

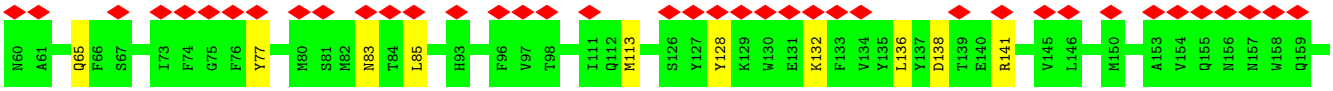


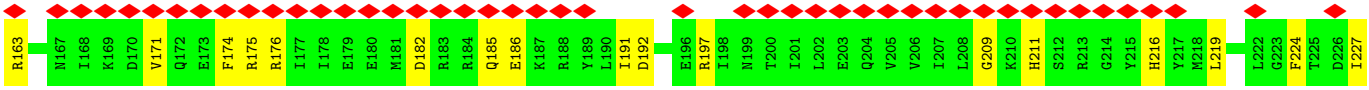


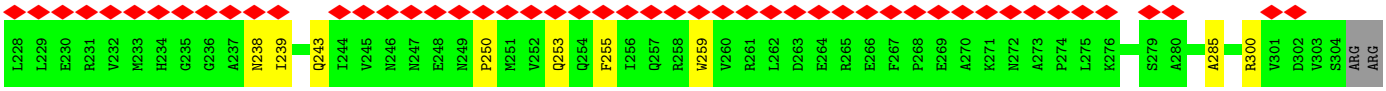
- Molecule 1: Glutamate receptor 3

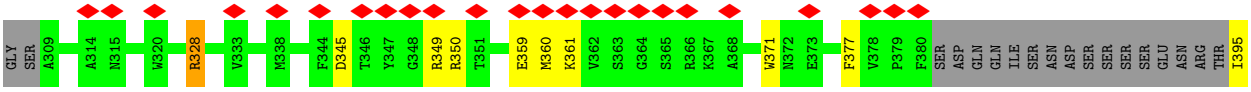
Chain C:

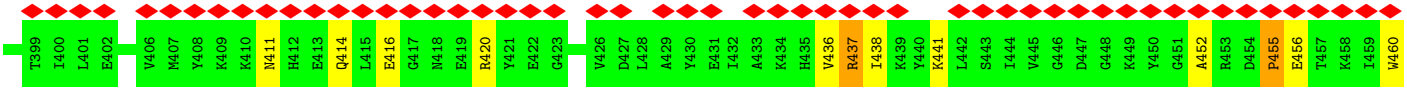


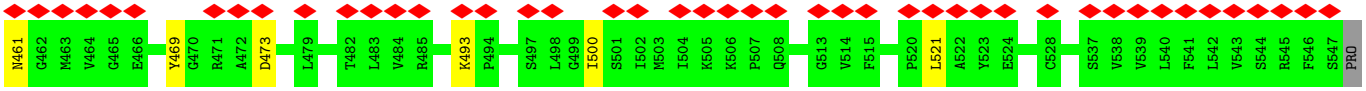


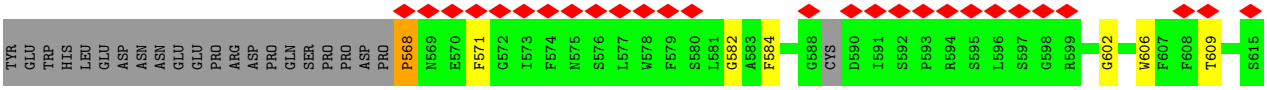


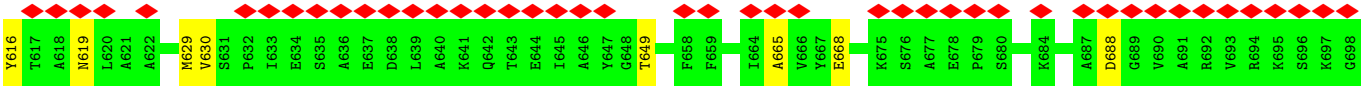


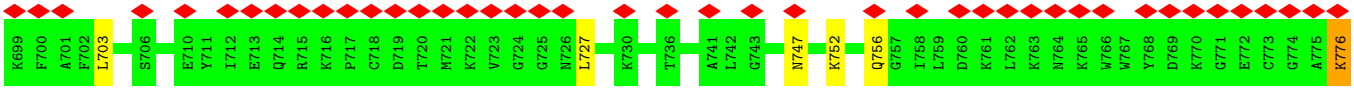


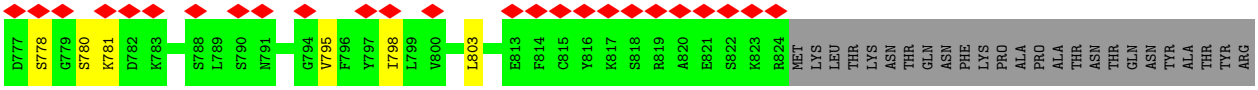












GLU GLY TYR ASN VAL TYR GLY THR GLU SER VAL LYS ILE

- Molecule 2: Glutamate receptor 2

Chain B: 47% 82% 6% 11%

MET GLN LYS ILE MET HIS ILE SER VAL LEU LEU SER PRO VAL LEU TRP GLY LEU ILE PHE GLY VAL SER SER N4 S5 I6 F12 P13 R14 Q18 E19 Y20 R24 V25 V28 S33 I41 D42 N43 L44 M48 S49 F50 A51 V52 T53 F56 Q59 F70

Y71 D72 K73 K74 N77 T78 I79 T80 S81 F82 C83 G84 T85 L86 H87 V88 S89 T92 P93 S94 F95 P96 G99 T100 H101 P102 F103 V104 I105 Q106 M107 G113 A114 L115 L116 S117 L118 I119 E120 Y121 Y122 Q123 W124 D125 K126 F127 A128 Y129 L130 R135 G136 L137 L140 Q141

A142 V143 L144 D145 S146 A147 A148 E149 K150 K151 W152 Q153 V154 T155 A156 I157 G160 N161 I162 N163 N164 D165 K166 K167 D168 E169 T170 Y171 R172 S173 L174 F175 Q176 D177 L178 E179 L180 K181 K182 E183 R184 R185 V186 I187 D193 K194 D197 I198 V199 D200 Q201 V202 I203 T204 I205 G206 K207

H208 V209 K210 G211 Y212 H213 Y214 I215 L219 L227 K228 I229 Q230 F231 G232 G233 A234 N235 V236 S237 I241 V242 D243 Y244 D245 D246 S247 S250 K251 F252 I253 E254 R255 W256 S257 T258 L259 E260 E261 K262 E263 Y264 P265 G266 A267 H268 I272 L278 A282 V283 K295 Q296

R297 I298 P313 A314 V315 P316 W317 G318 Q319 G320 V321 E322 I323 E324 R325 A326 L327 K328 Q329 D342 Q343 N344 G345 K346 R347 I348 N349 N353 I354 M355 E356 L357 K358 T359 N360 G361 P362 R363 K364 I365 G366 Y367 W368 S369 E370 V371 D372 K373 M374 V375 V376 T377 L378 THR GLU LEU PRO

SER GLY ASN ASP THR SER GLY LEU GLU ASN LYS THR V395 I400 L401 E402 S403 P404 Y405 M408 K409 K410 N411 H412 E413 M414 N418 Y424 A429 A430 E431 I432 A433 K434 D447 G448 K449 Y450 G451 A452 R453 D454 A455 D456 T457 K458 I459 W460 N461 A472 P478 L479

T480 I481 F491 S492 K493 P494 F495 M496 S497 L498 G499 I500 S501 I502 M503 I504 K505 K506 P507 Q508 K509 S510 K511 P512 G513 V514 F515 S516 F517 L518 D519 P520 L521 A522 Y523 E524 I525 W526 M527 C528 I529 V530 F531 A532 Y533 V539 L540 S544 R545 F546 S547 P548 TYR GLU TRP HIS THR

GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR N569 E570 F571 G572 G582 R586 Q587 GLY CYS ASP I591 S592 P593 R594 S595 L596 R599 I600 W606 L610 I611 I612 S615 N619 L620 A621 A622 F623 L624 T625 V626 E627 R628 M629 V630 S631 P632 I633

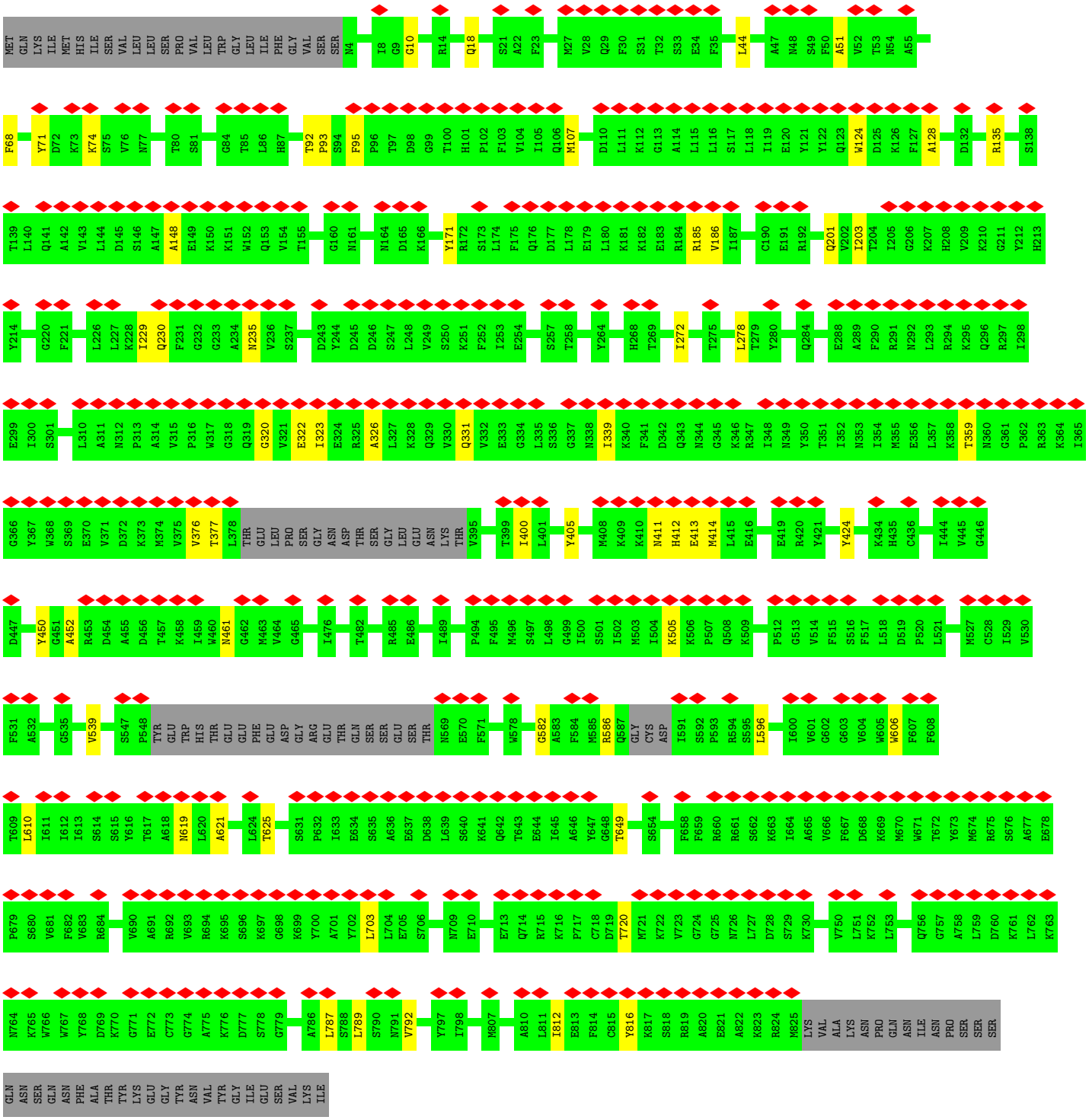
E634 S635 A636 E637 D638 L639 S640 K641 Q642 T643 E644 I645 A646 Y647 G648 T649 R661 S662 K663 I664 A665 V666 F667 D668 K669 M670 W671 T672 Y673 M674 R675 S676 A677 E678 P679 S680 A691 R692 K695 S696 K697 G698 K699 Y700 L703 K716 P717 C718 D719 D728 S729 G739 S740

A744 W747 L748 A749 V750 L751 K752 L753 Q756 G757 A758 L759 D760 K761 L762 K763 N764 Y768 G774 A775 K776 D777 S778 G779 S780 K781 E782 K783 T784 L787 S788 L789 V792 A793 G794 V795 F796 Y797 T798 L799 V800 G801 G802 L803 G804 L805 A806 M807 L808 V809 I812 E813

Y816 K817 S818 R819 A820 E821 A822 K823 R824 M825 LYS VAL ALA LYS ASN PRO GLN ASN ILE ASN PRO SER SER SER GLN ASN SER GLN ASN PHE ALA THR TYR LYS GLU GLY TYR ASN VAL TYR GLY ILE GLU SER VAL LYS ILE

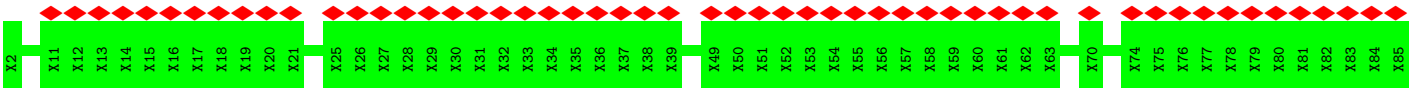
- Molecule 2: Glutamate receptor 2

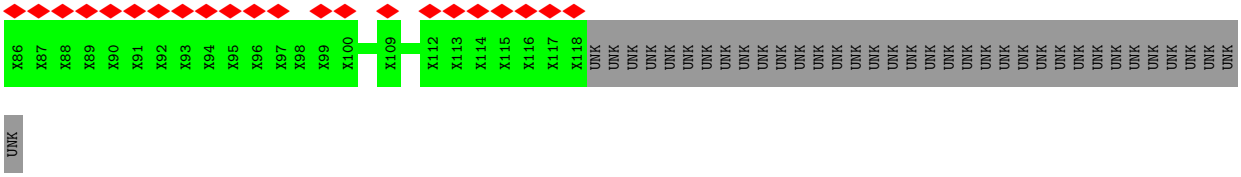
Chain D: 50% 82% 7% 11%



- Molecule 3: A'-C' auxiliary proteins

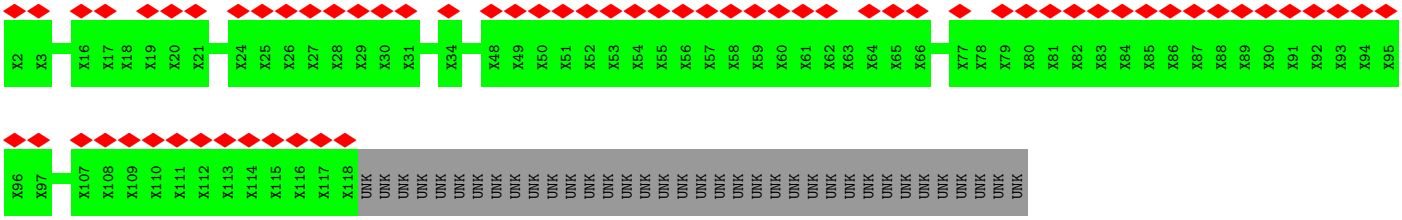
Chain E:





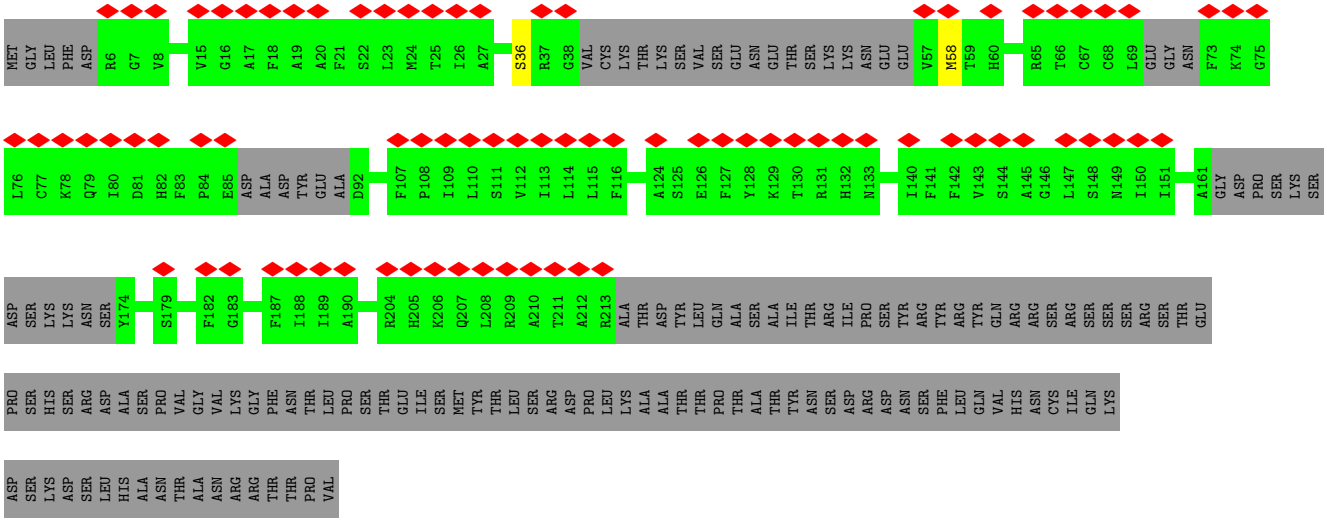
• Molecule 3: A'-C' auxiliary proteins

Chain G:



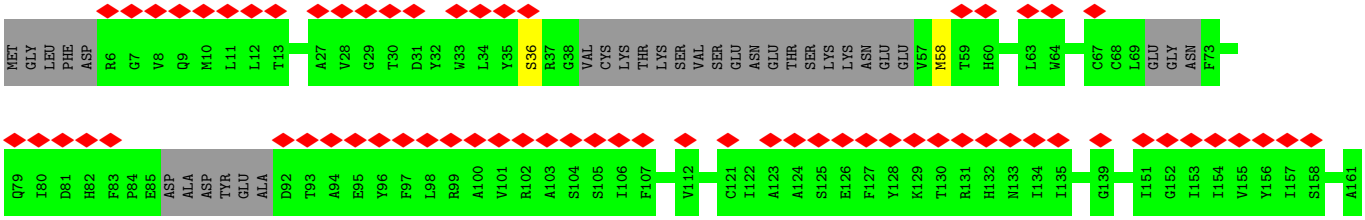
• Molecule 4: Voltage-dependent calcium channel gamma-2 subunit

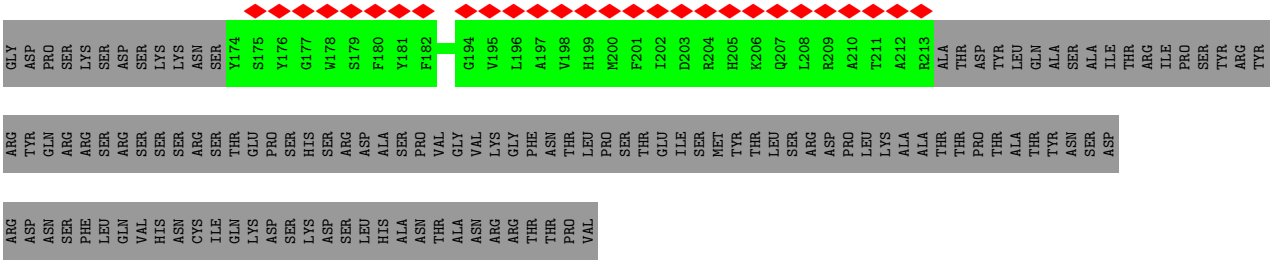
Chain F:



• Molecule 4: Voltage-dependent calcium channel gamma-2 subunit

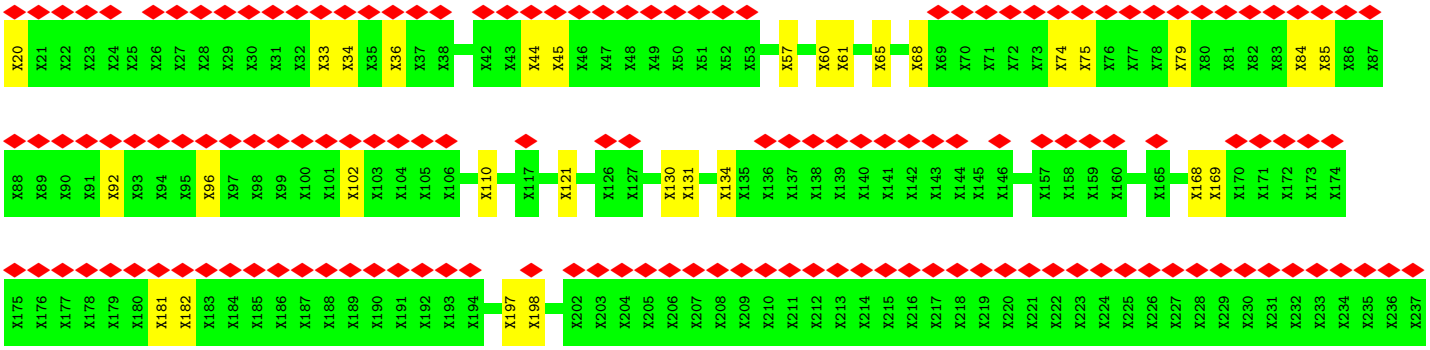
Chain H:





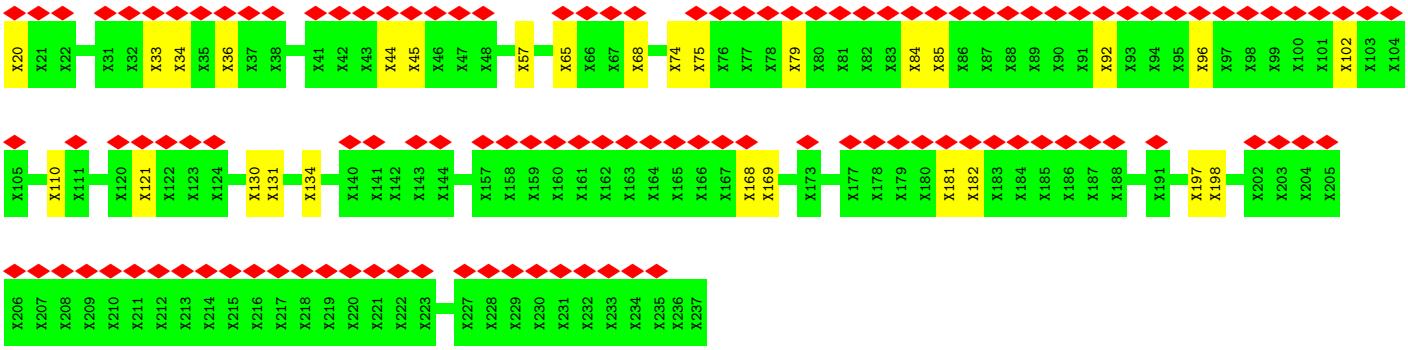
- Molecule 5: 5B2 Fab Light Chain

Chain I:



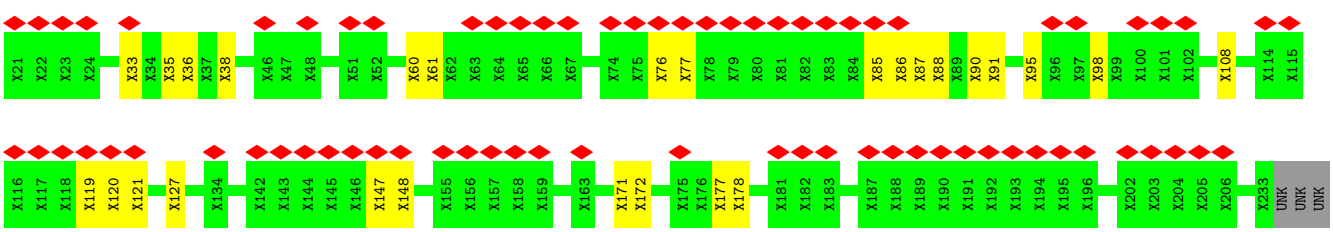
- Molecule 5: 5B2 Fab Light Chain

Chain M:



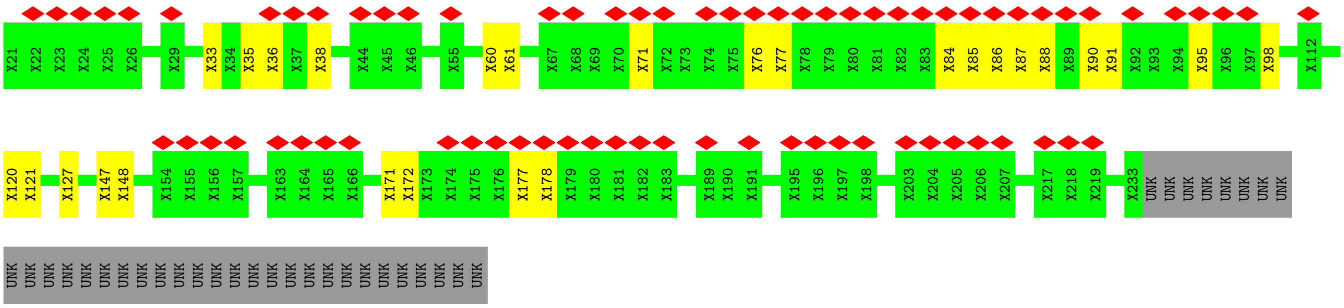
- Molecule 6: 5B2 Fab Heavy Chain

Chain J:



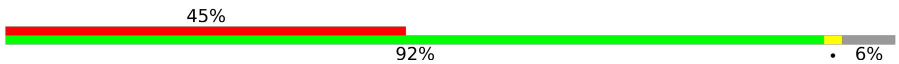
- Molecule 6: 5B2 Fab Heavy Chain

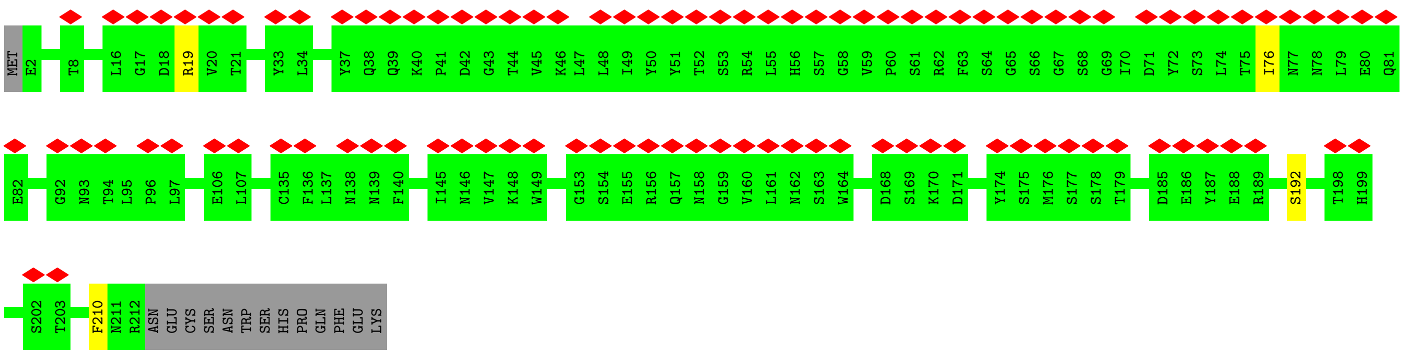
Chain N:



- Molecule 7: 15F1 Fab light chain

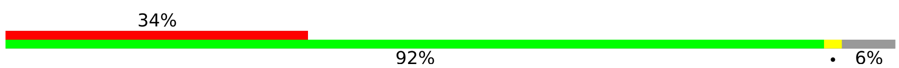
Chain K:

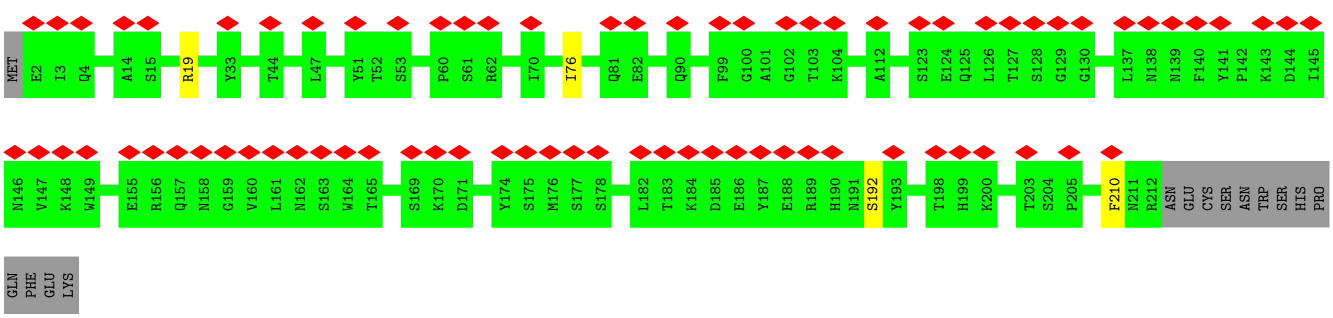




- Molecule 7: 15F1 Fab light chain

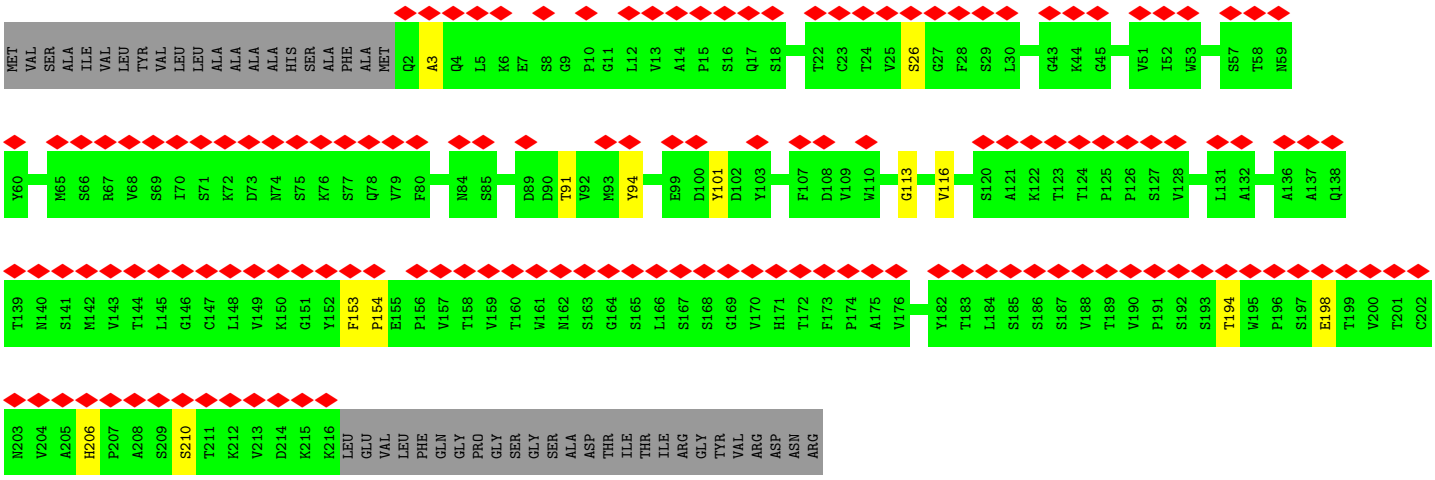
Chain O:





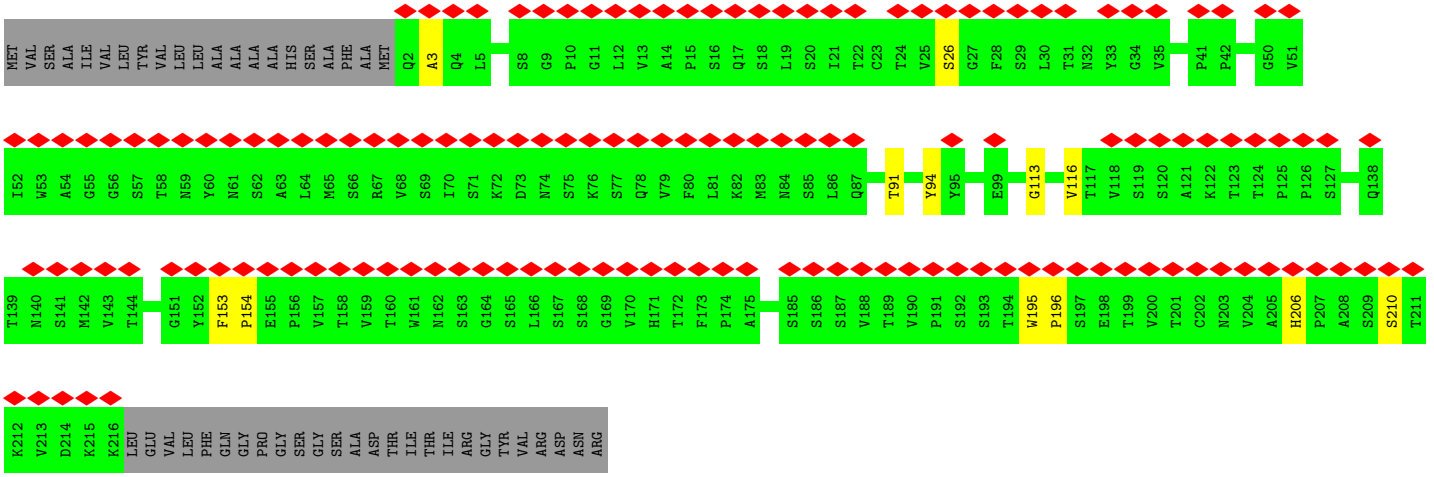
- Molecule 8: 15F1 Fab heavy chain

Chain L:



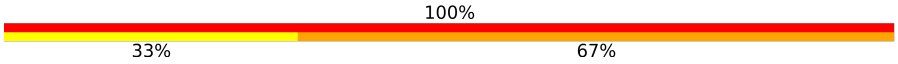
• Molecule 8: 15F1 Fab heavy chain

Chain P:



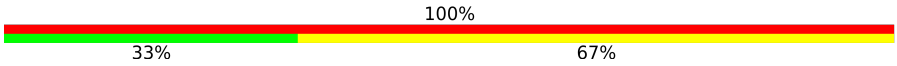
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

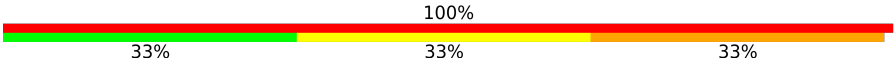
Chain S:



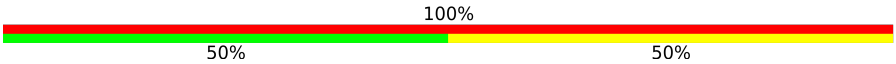
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99000	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, ZK1

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	0/6149	0.49	5/8360 (0.1%)
1	C	0.28	0/6149	0.49	5/8360 (0.1%)
2	B	0.26	0/5809	0.48	1/7950 (0.0%)
2	D	0.26	0/5805	0.48	1/7946 (0.0%)
4	F	0.27	0/1021	0.41	0/1401
4	H	0.27	0/1021	0.42	0/1401
7	K	0.25	0/1041	0.47	0/1448
7	O	0.25	0/1041	0.47	0/1448
8	L	0.26	0/1058	0.50	0/1470
8	P	0.26	0/1058	0.50	0/1470
All	All	0.27	0/30152	0.48	12/41254 (0.0%)

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
2	D	0	1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455	PRO	CA-N-CD	-8.64	99.41	111.50
1	C	455	PRO	CA-N-CD	-8.61	99.45	111.50
1	A	568	PRO	CA-N-CD	-8.54	99.55	111.50
1	C	568	PRO	CA-N-CD	-8.51	99.58	111.50
1	A	3	PRO	C-N-CA	6.59	138.18	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	235	ASN	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	6011	0	5715	78	0
1	C	6011	0	5713	84	0
2	B	5684	0	5206	39	0
2	D	5680	0	5195	39	0
3	E	585	0	125	0	0
3	G	585	0	125	0	0
4	F	1007	0	718	1	0
4	H	1007	0	718	1	0
5	I	1090	0	232	18	0
5	M	1090	0	233	17	0
6	J	1065	0	223	15	0
6	N	1065	0	226	15	0
7	K	1042	0	453	2	0
7	O	1042	0	453	2	0
8	L	1059	0	470	9	0
8	P	1059	0	470	8	0
9	Q	39	0	34	2	0
9	S	39	0	34	0	0
9	T	39	0	34	0	0
9	V	39	0	34	1	0
10	R	28	0	25	0	0
10	U	28	0	25	2	0
11	A	27	0	13	1	0
11	B	27	0	13	1	0
11	C	27	0	13	0	0
11	D	27	0	13	1	0
12	A	14	0	13	0	0
12	B	14	0	13	0	0
12	C	14	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	14	0	13	0	0
All	All	35458	0	26564	316	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 5.

The worst 5 of 316 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:A:185:GLN:CG	1:A:469:TYR:CE1	1.84	1.60
1:A:185:GLN:HG2	1:A:469:TYR:CE1	1.36	1.52
1:C:185:GLN:CG	1:C:469:TYR:CE1	1.93	1.50
1:C:185:GLN:CD	1:C:469:TYR:HE1	1.13	1.44
1:A:185:GLN:CG	1:A:469:TYR:HE1	1.16	1.41

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	774/888 (87%)	737 (95%)	35 (4%)	2 (0%)	41 76
1	C	774/888 (87%)	737 (95%)	35 (4%)	2 (0%)	41 76
2	B	775/883 (88%)	735 (95%)	40 (5%)	0	100 100
2	D	775/883 (88%)	736 (95%)	39 (5%)	0	100 100
4	F	159/323 (49%)	156 (98%)	3 (2%)	0	100 100
4	H	159/323 (49%)	156 (98%)	3 (2%)	0	100 100
7	K	209/225 (93%)	202 (97%)	7 (3%)	0	100 100
7	O	209/225 (93%)	203 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	L	213/262 (81%)	210 (99%)	3 (1%)	0	100	100
8	P	213/262 (81%)	211 (99%)	2 (1%)	0	100	100
All	All	4260/5162 (82%)	4083 (96%)	173 (4%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ARG
1	A	778	SER
1	C	437	ARG
1	C	778	SER

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	617/766 (80%)	612 (99%)	5 (1%)	81	89
1	C	617/766 (80%)	613 (99%)	4 (1%)	86	92
2	B	552/753 (73%)	549 (100%)	3 (0%)	88	93
2	D	551/753 (73%)	549 (100%)	2 (0%)	91	94
4	F	50/275 (18%)	50 (100%)	0	100	100
4	H	50/275 (18%)	50 (100%)	0	100	100
All	All	2437/3588 (68%)	2423 (99%)	14 (1%)	86	92

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	619	ASN
1	C	176	ARG
2	D	619	ASN
1	C	776	LYS
2	D	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	18	GLN
1	C	756	GLN
1	C	20	HIS
1	C	343	GLN
2	B	619	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)

16 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	$\#\|Z\| > 2$
9	NAG	Q	1	9,1	14,14,15	0.97	1 (7%)	17,19,21	2.39	4 (23%)
9	NAG	Q	2	9	14,14,15	0.51	0	17,19,21	0.46	0
9	BMA	Q	3	9	11,11,12	0.80	0	15,15,17	0.88	1 (6%)
10	NAG	R	1	10,1	14,14,15	0.49	0	17,19,21	0.62	0
10	NAG	R	2	10	14,14,15	0.65	0	17,19,21	0.96	1 (5%)
9	NAG	S	1	9,2	14,14,15	1.33	2 (14%)	17,19,21	2.66	4 (23%)
9	NAG	S	2	9	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
9	BMA	S	3	9	11,11,12	0.80	0	15,15,17	0.74	0
9	NAG	T	1	9,1	14,14,15	1.06	1 (7%)	17,19,21	2.53	5 (29%)
9	NAG	T	2	9	14,14,15	0.70	0	17,19,21	0.60	0
9	BMA	T	3	9	11,11,12	0.80	0	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	U	1	10,1	14,14,15	0.36	0	17,19,21	0.65	0
10	NAG	U	2	10	14,14,15	0.32	0	17,19,21	0.51	0
9	NAG	V	1	9,2	14,14,15	0.50	0	17,19,21	0.43	0
9	NAG	V	2	9	14,14,15	1.16	2 (14%)	17,19,21	1.38	3 (17%)
9	BMA	V	3	9	11,11,12	0.89	0	15,15,17	0.73	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
9	NAG	Q	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	1/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	0/2/19/22	0/1/1/1
10	NAG	R	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	R	2	10	-	3/6/23/26	0/1/1/1
9	NAG	S	1	9,2	-	5/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	0/2/19/22	0/1/1/1
9	NAG	T	1	9,1	-	5/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	1/6/23/26	0/1/1/1
9	NAG	V	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	3/6/23/26	0/1/1/1
9	BMA	V	3	9	-	1/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	1	NAG	O5-C1	3.84	1.49	1.43
9	T	1	NAG	O5-C1	-3.39	1.38	1.43
9	V	2	NAG	O5-C1	-3.30	1.38	1.43
9	Q	1	NAG	O5-C1	-2.90	1.39	1.43
9	S	1	NAG	C1-C2	2.38	1.55	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	1	NAG	C2-N2-C7	8.07	134.39	122.90
9	S	1	NAG	C2-N2-C7	7.96	134.23	122.90
9	Q	1	NAG	C2-N2-C7	7.92	134.19	122.90
9	S	1	NAG	C1-O5-C5	5.70	119.92	112.19
9	T	1	NAG	C1-C2-N2	3.86	117.08	110.49

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	T	1	NAG	O5-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
10	R	2	NAG	C4-C5-C6-O6
9	Q	1	NAG	C8-C7-N2-C2
9	Q	1	NAG	O7-C7-N2-C2

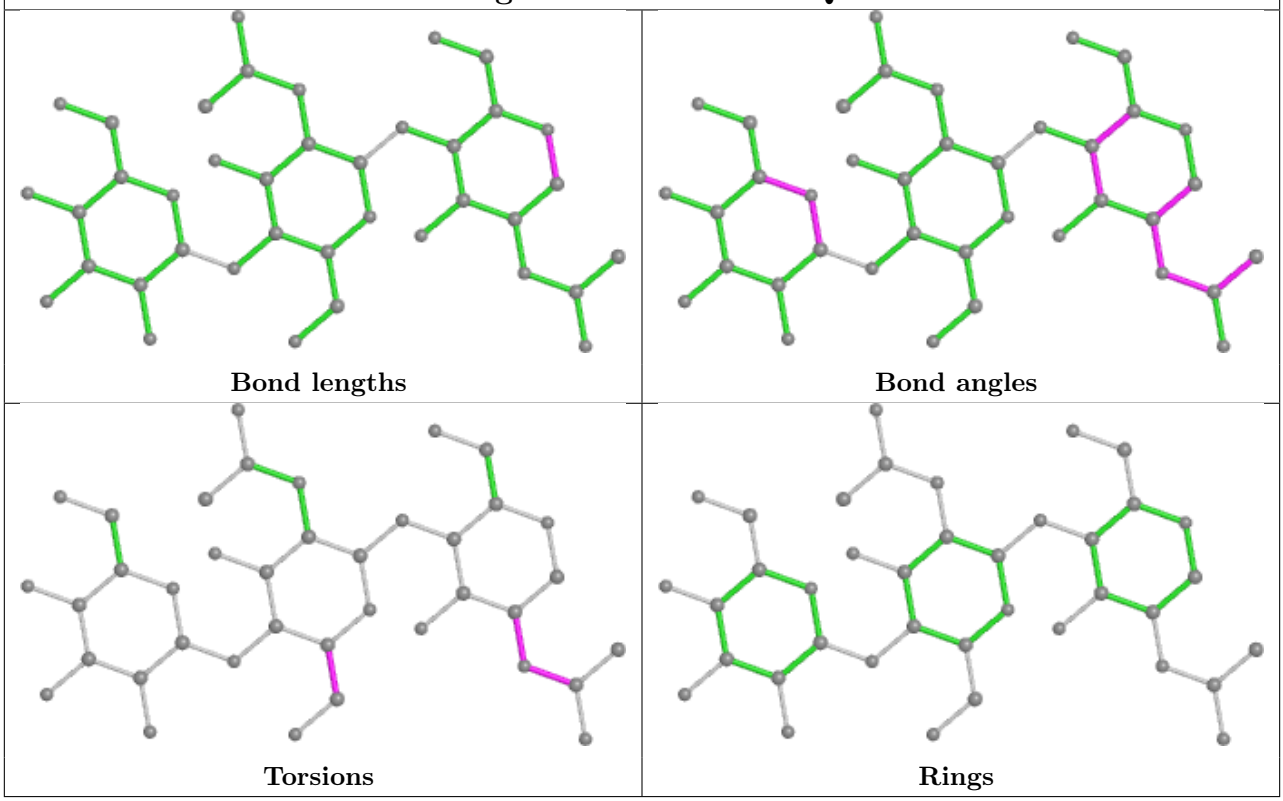
There are no ring outliers.

6 monomers are involved in 5 short contacts:

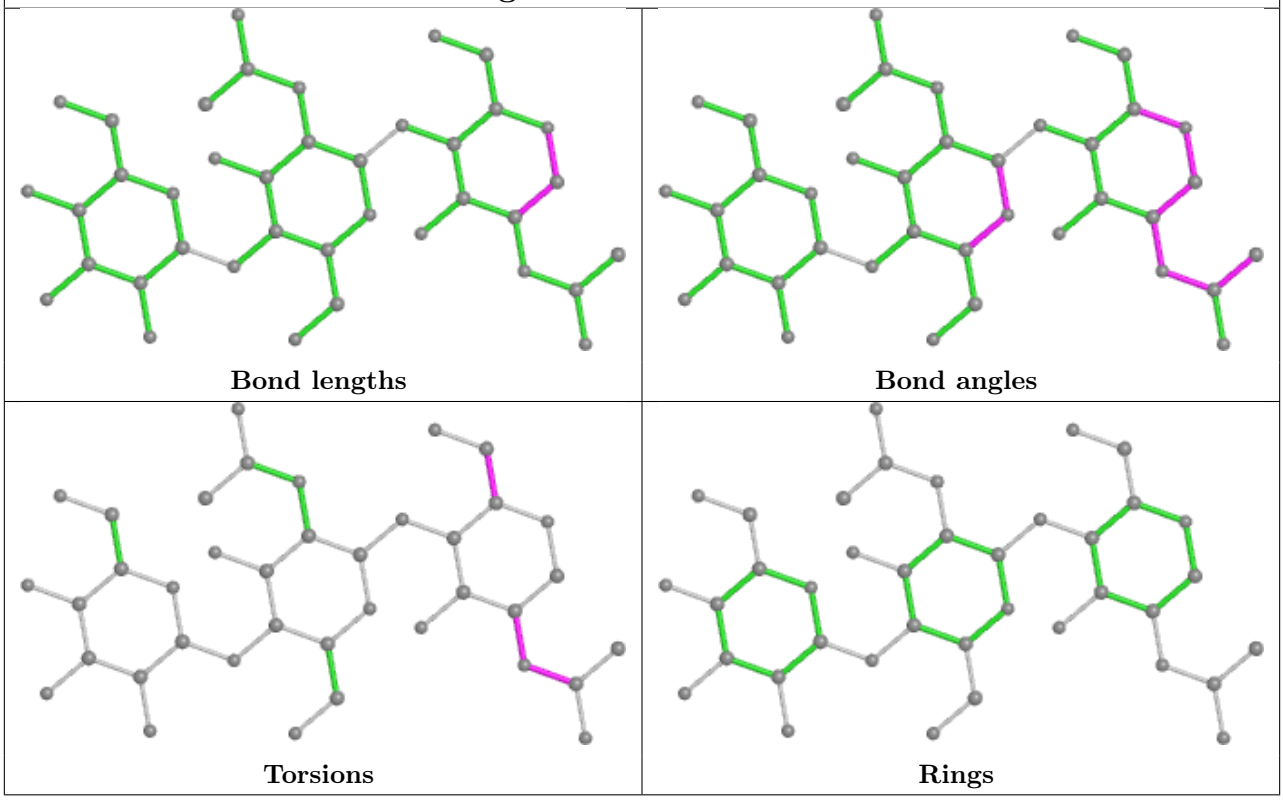
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	2	NAG	2	0
9	Q	1	NAG	1	0
10	U	1	NAG	2	0
9	Q	3	BMA	1	0
9	V	1	NAG	1	0
9	V	2	NAG	1	0

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

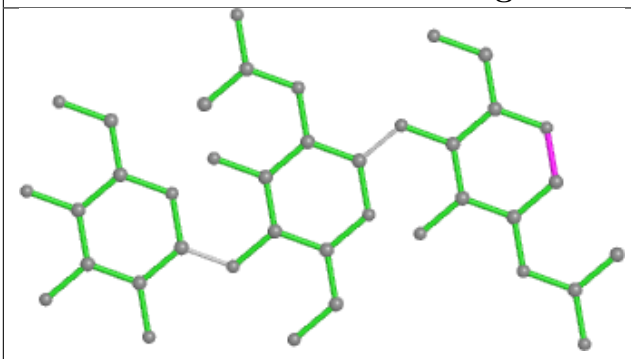
Oligosaccharide Chain Q



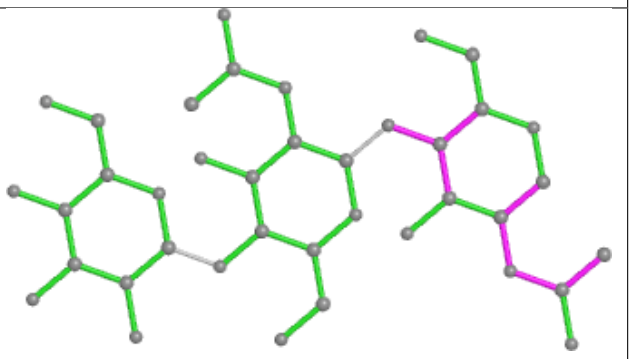
Oligosaccharide Chain S



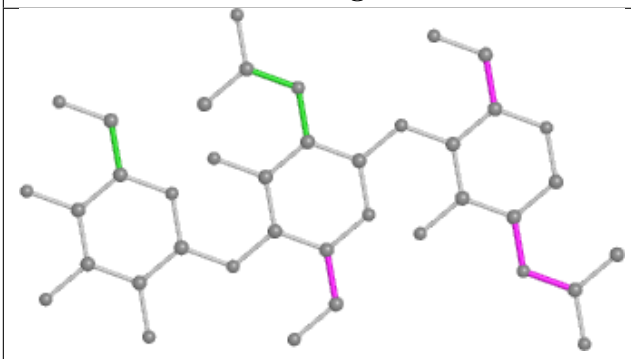
Oligosaccharide Chain T



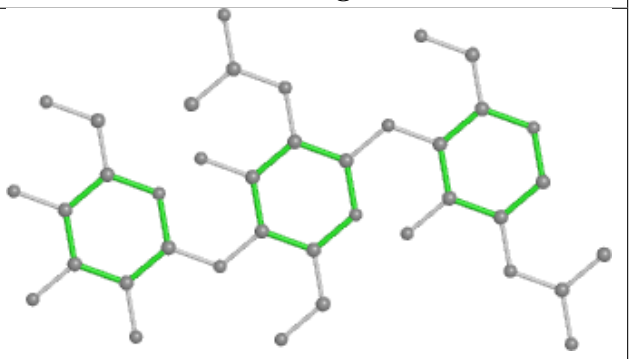
Bond lengths



Bond angles

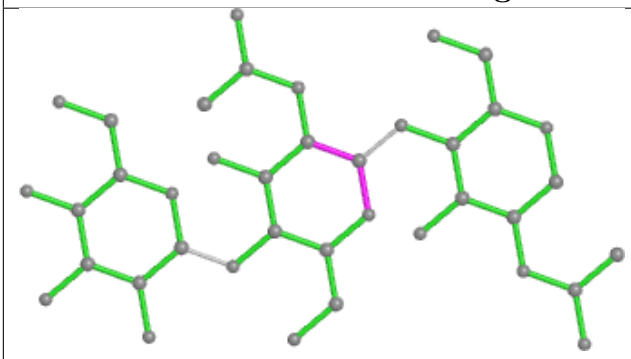


Torsions

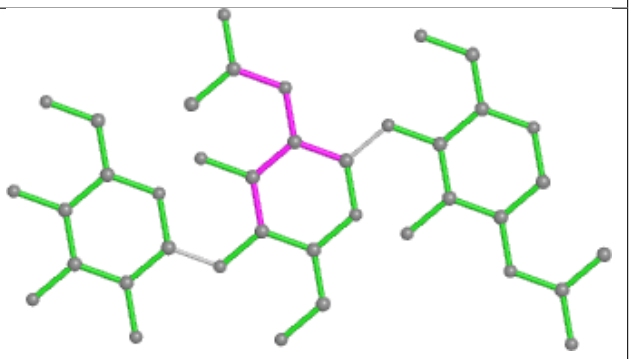


Rings

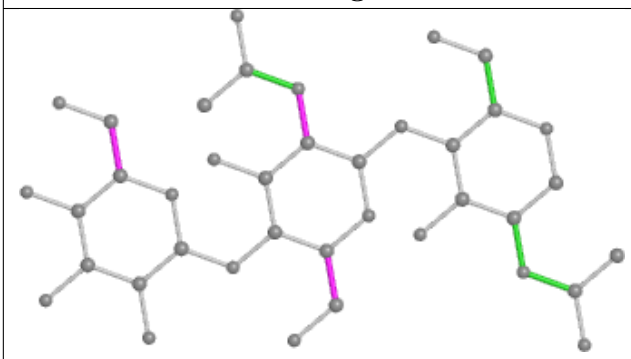
Oligosaccharide Chain V



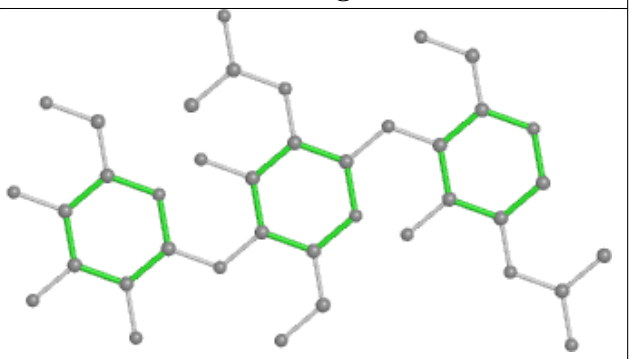
Bond lengths



Bond angles

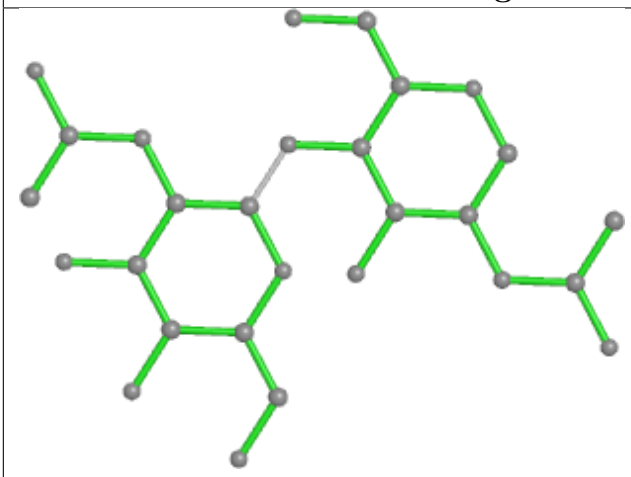


Torsions

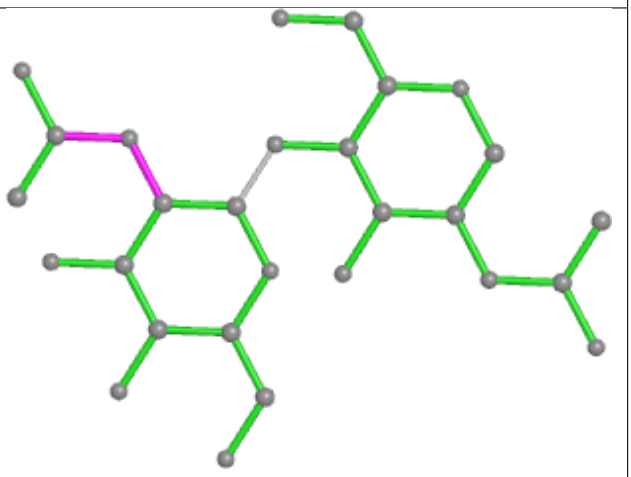


Rings

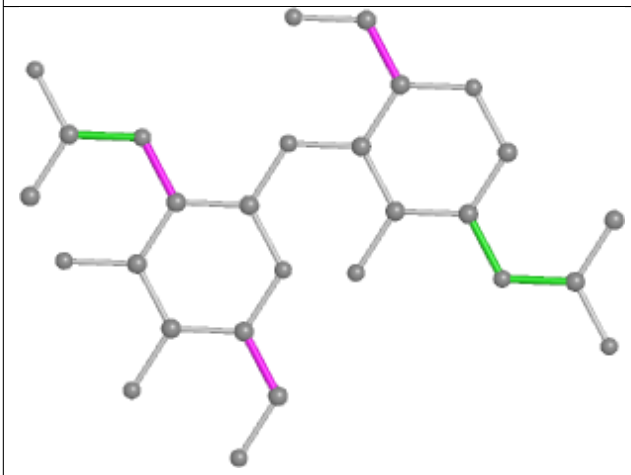
Oligosaccharide Chain R



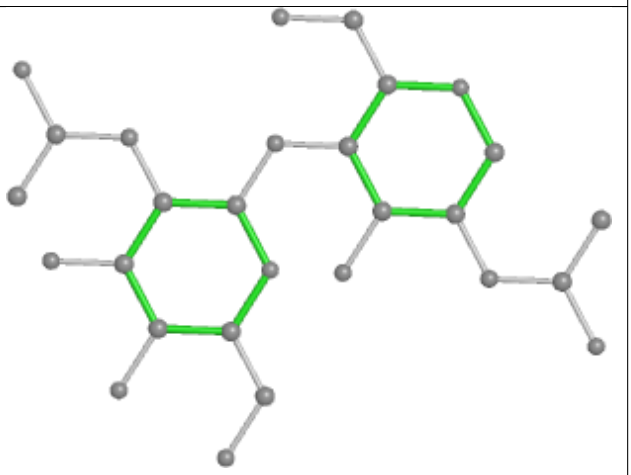
Bond lengths



Bond angles

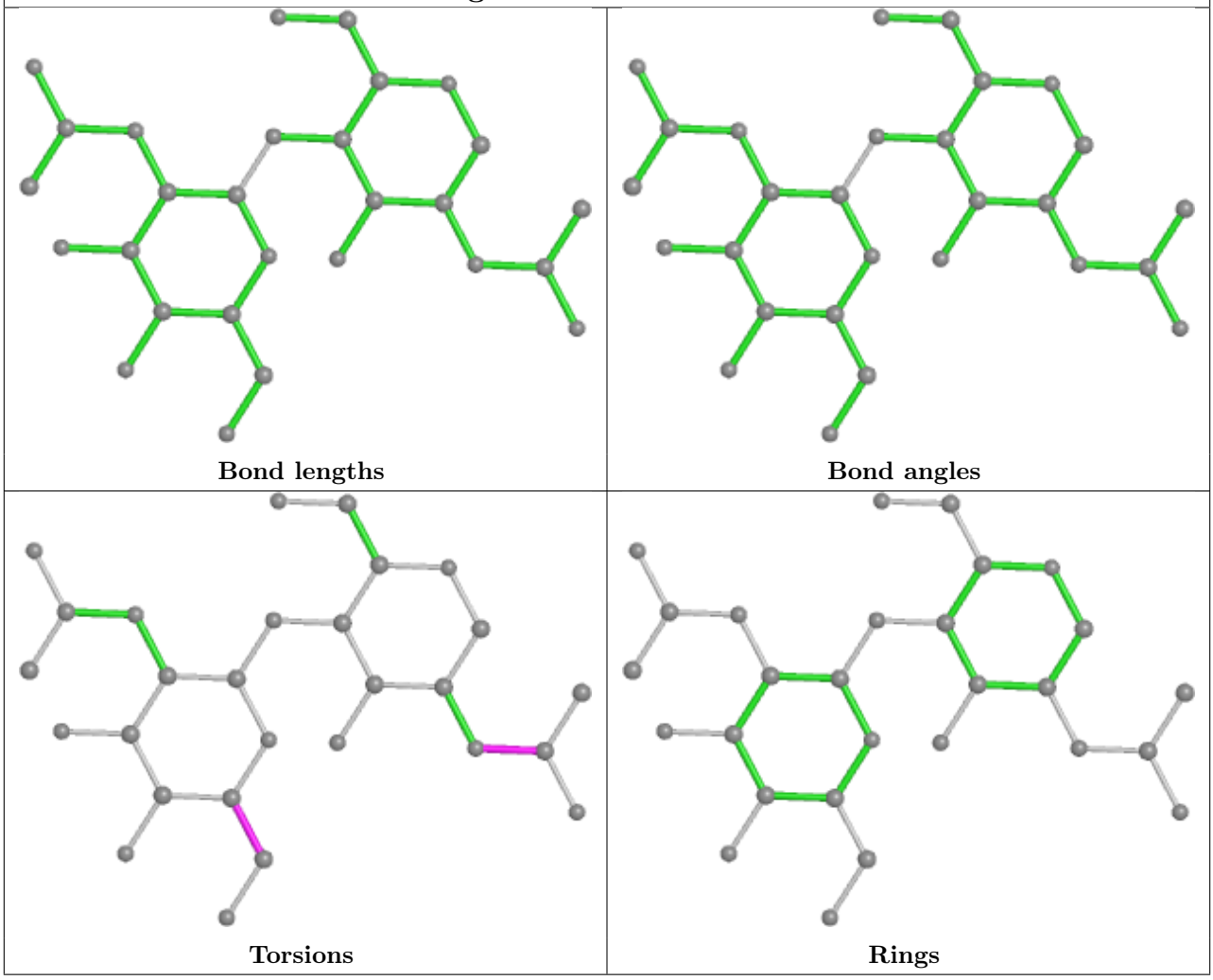


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
11	ZK1	D	901	-	28,29,29	2.73	9 (32%)	42,45,45	1.73	9 (21%)
11	ZK1	A	901	-	28,29,29	2.74	9 (32%)	42,45,45	1.66	9 (21%)
12	NAG	A	905	1	14,14,15	0.41	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ZK1	B	901	-	28,29,29	2.74	9 (32%)	42,45,45	1.74	9 (21%)
11	ZK1	C	901	-	28,29,29	2.73	9 (32%)	42,45,45	1.65	9 (21%)
12	NAG	D	905	2	14,14,15	0.37	0	17,19,21	0.52	0
12	NAG	C	905	1	14,14,15	0.31	0	17,19,21	0.44	0
12	NAG	B	905	2	14,14,15	0.32	0	17,19,21	0.48	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
11	ZK1	D	901	-	-	5/13/23/23	0/3/3/3
11	ZK1	A	901	-	-	3/13/23/23	0/3/3/3
12	NAG	A	905	1	-	2/6/23/26	0/1/1/1
11	ZK1	B	901	-	-	5/13/23/23	0/3/3/3
11	ZK1	C	901	-	-	3/13/23/23	0/3/3/3
12	NAG	D	905	2	-	0/6/23/26	0/1/1/1
12	NAG	C	905	1	-	0/6/23/26	0/1/1/1
12	NAG	B	905	2	-	1/6/23/26	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	901	ZK1	OAA-CAT	8.84	1.40	1.23
11	A	901	ZK1	OAA-CAT	8.84	1.40	1.23
11	C	901	ZK1	OAA-CAT	8.83	1.40	1.23
11	B	901	ZK1	OAA-CAT	8.80	1.40	1.23
11	B	901	ZK1	OAB-CAU	8.32	1.40	1.23

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	901	ZK1	CAN-NAX-CAM	4.79	122.08	111.52
11	D	901	ZK1	CAN-NAX-CAM	4.70	121.89	111.52
11	C	901	ZK1	CAN-NAX-CAM	4.06	120.48	111.52
11	A	901	ZK1	CAN-NAX-CAM	4.05	120.45	111.52
11	A	901	ZK1	CAV-NAP-CAT	-3.82	119.94	124.80

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

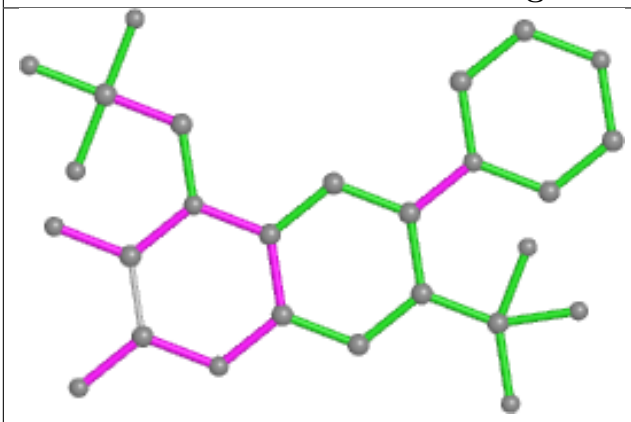
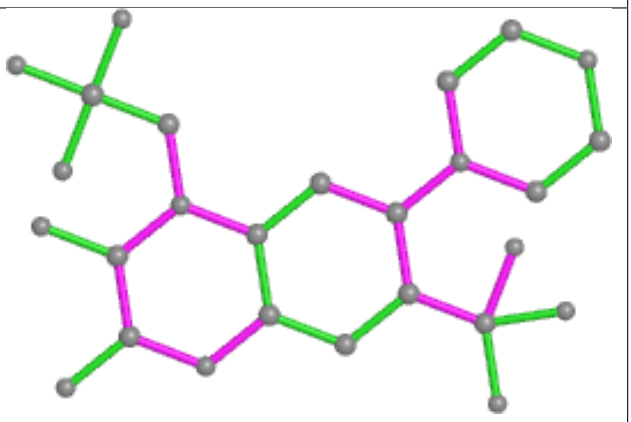
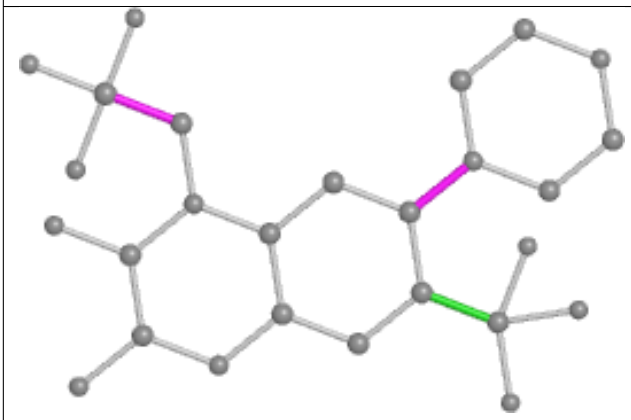
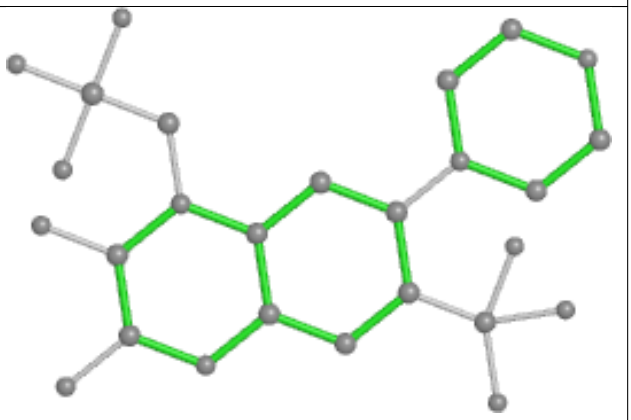
Mol	Chain	Res	Type	Atoms
11	B	901	ZK1	NAY-CAO-PBA-OAD
11	B	901	ZK1	NAY-CAO-PBA-OAE
11	D	901	ZK1	NAY-CAO-PBA-OAD
11	D	901	ZK1	NAY-CAO-PBA-OAE
12	A	905	NAG	C4-C5-C6-O6

There are no ring outliers.

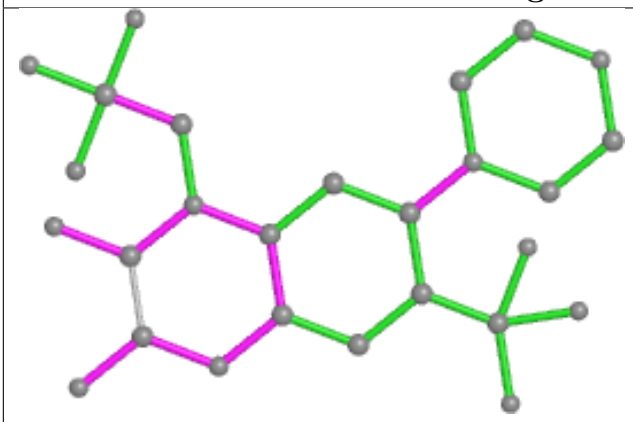
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	901	ZK1	1	0
11	A	901	ZK1	1	0
11	B	901	ZK1	1	0

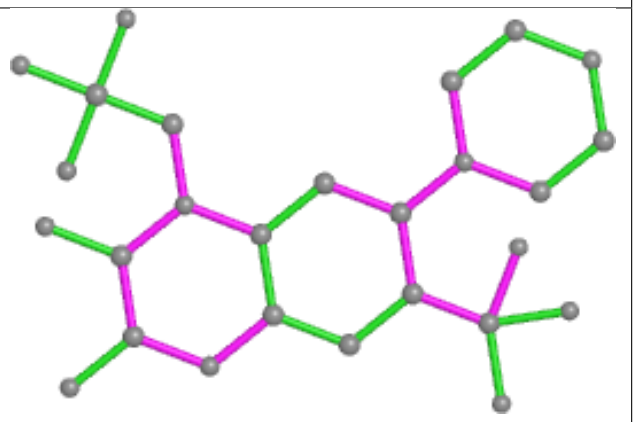
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ZK1 D 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

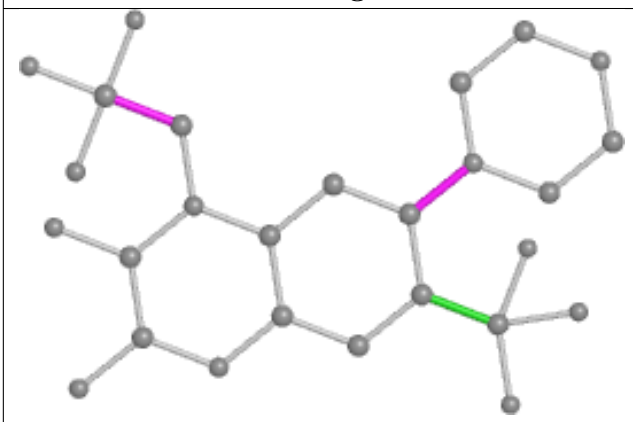
Ligand ZK1 A 901



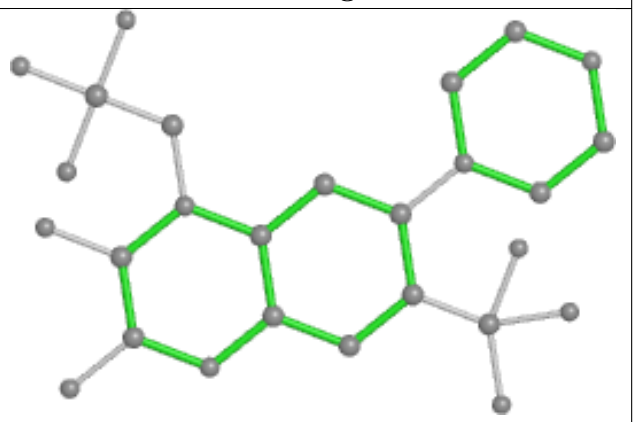
Bond lengths



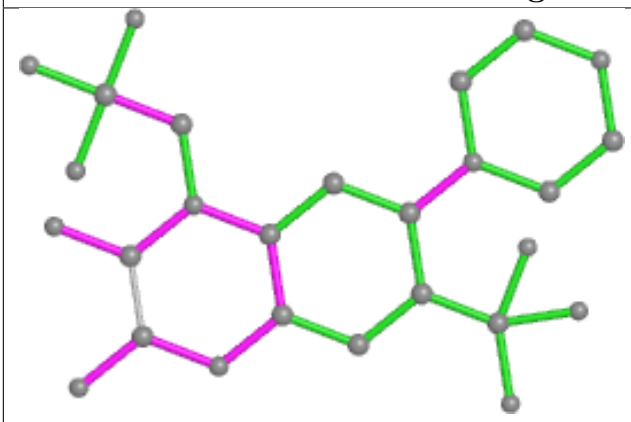
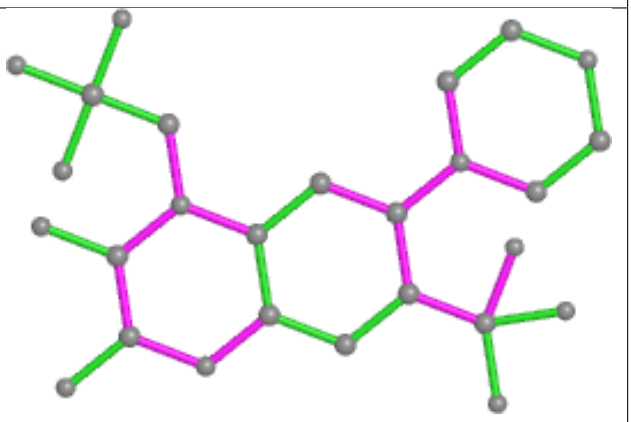
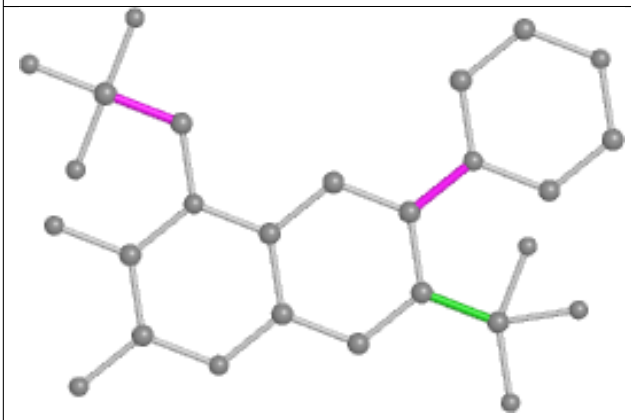
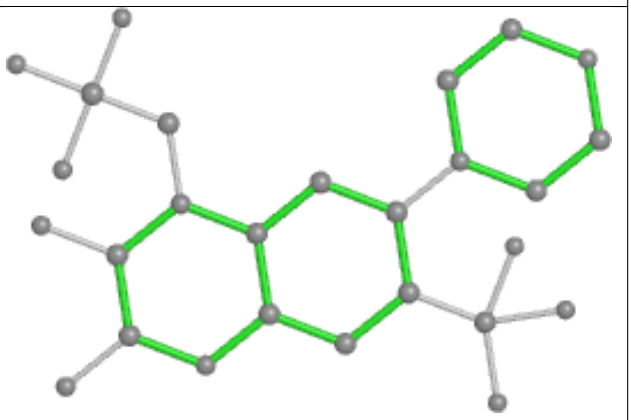
Bond angles



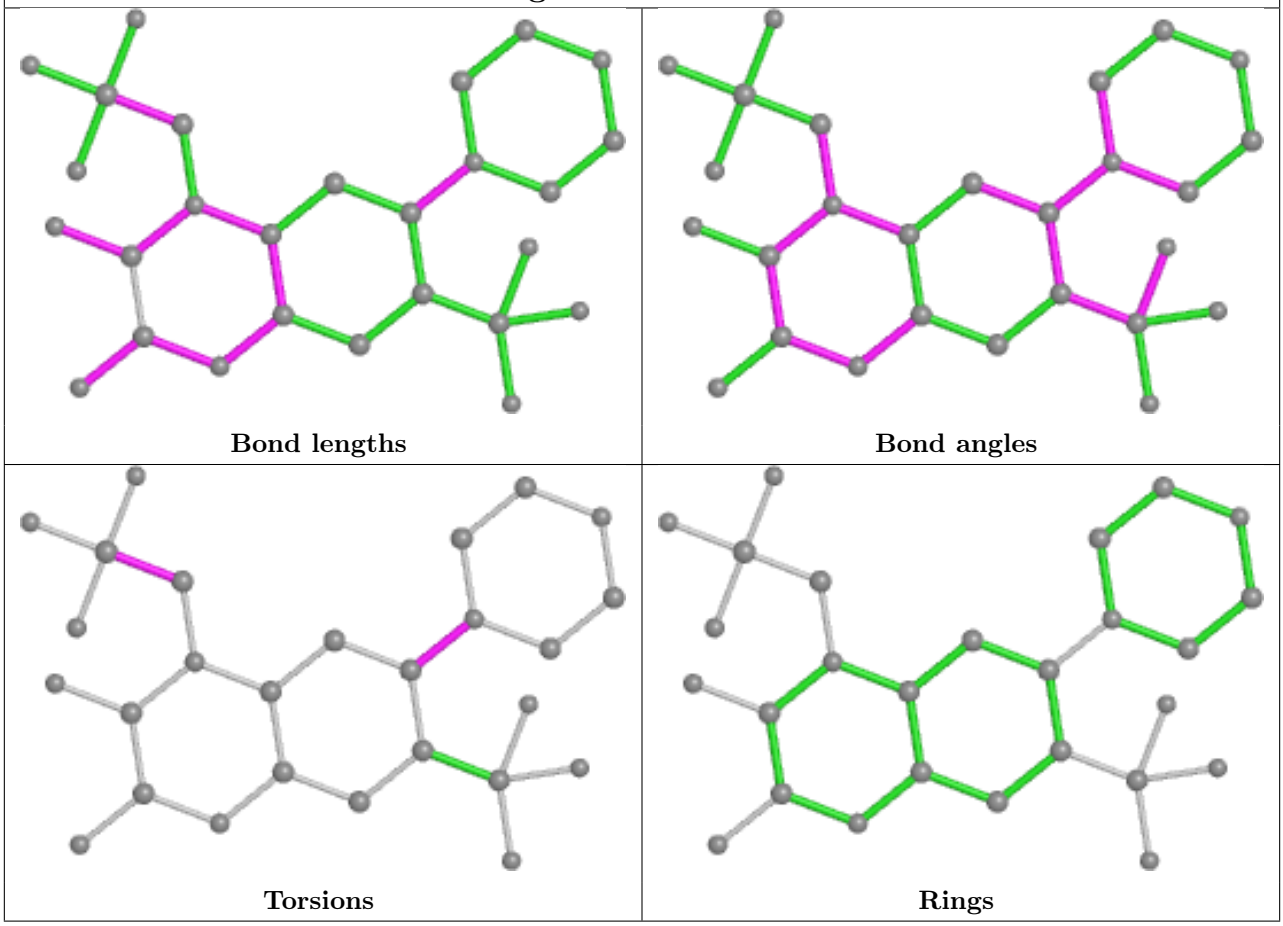
Torsions



Rings

Ligand ZK1 B 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZK1 C 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	3
3	E	3

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	21:UNK	C	22:UNK	N	14.88
1	G	55:UNK	C	56:UNK	N	14.61
1	E	55:UNK	C	56:UNK	N	14.51

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	21:UNK	C	22:UNK	N	14.49
1	G	88:UNK	C	89:UNK	N	13.73

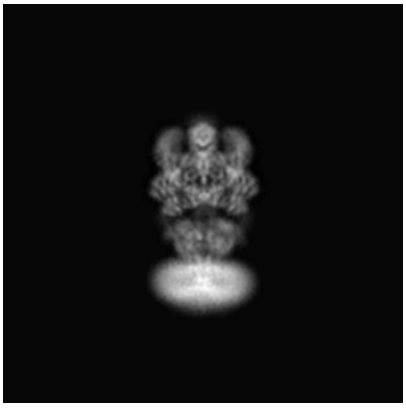
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9388. These allow visual inspection of the internal detail of the map and identification of artifacts.

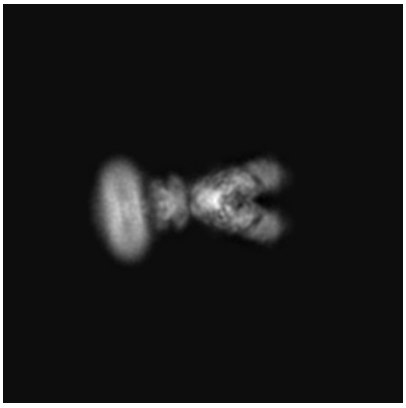
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

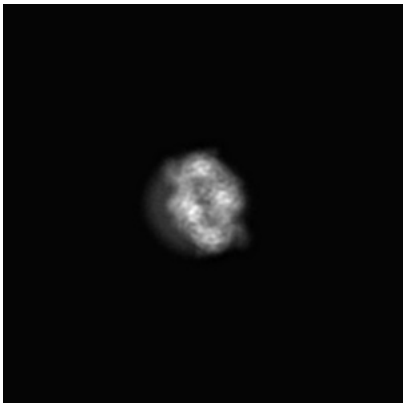
6.1.1 Primary map



X



Y



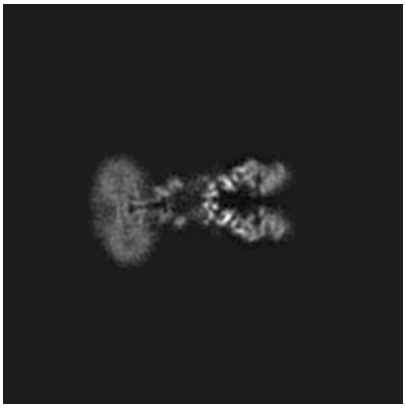
Z

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

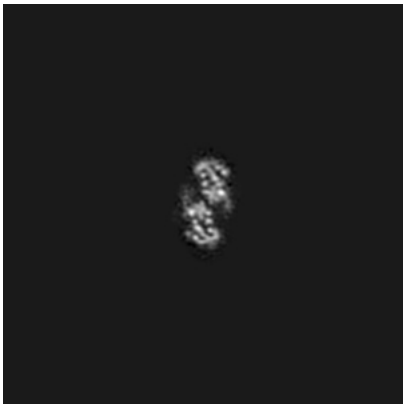
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160



Y Index: 160



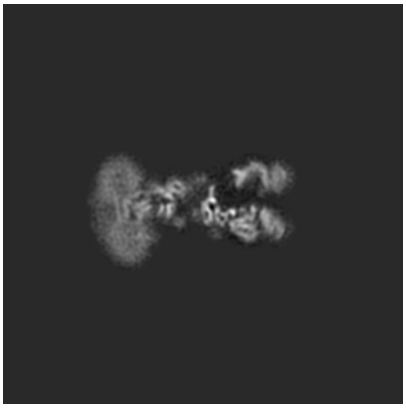
Z Index: 160

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

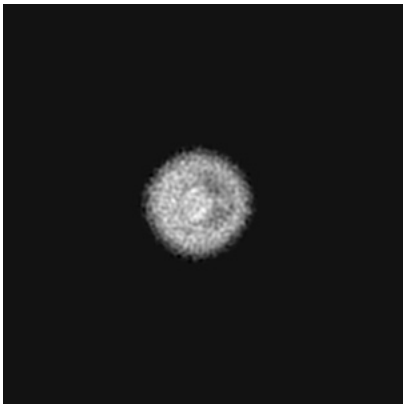
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 157



Y Index: 157

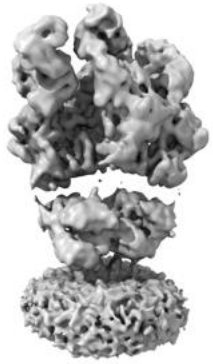


Z Index: 91

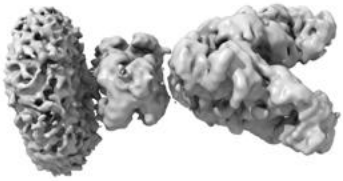
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

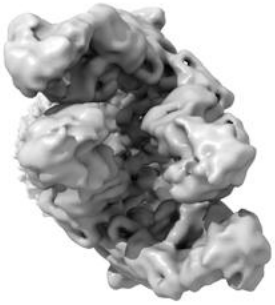
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

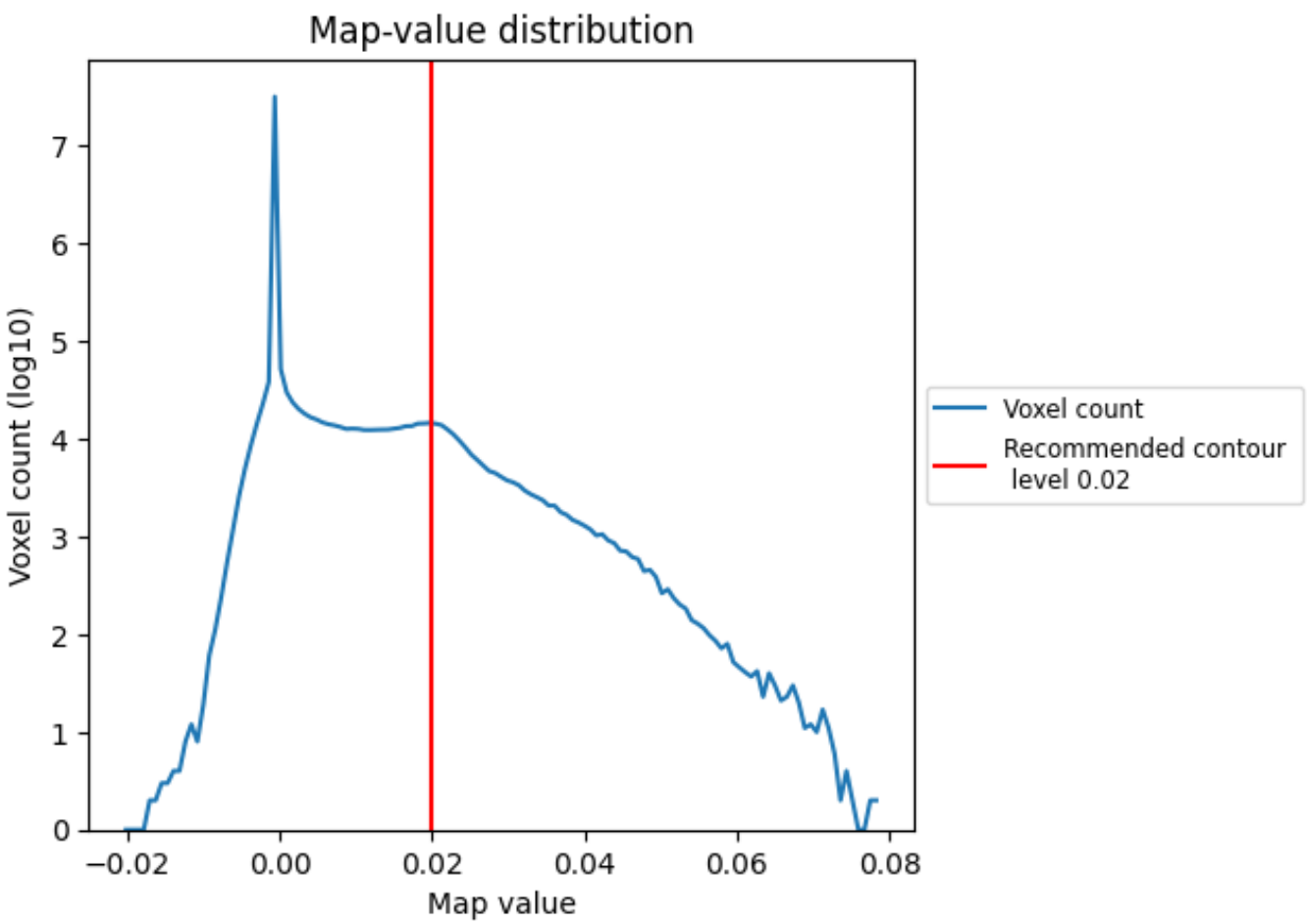
6.5 Mask visualisation (i)

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

7 Map analysis (i)

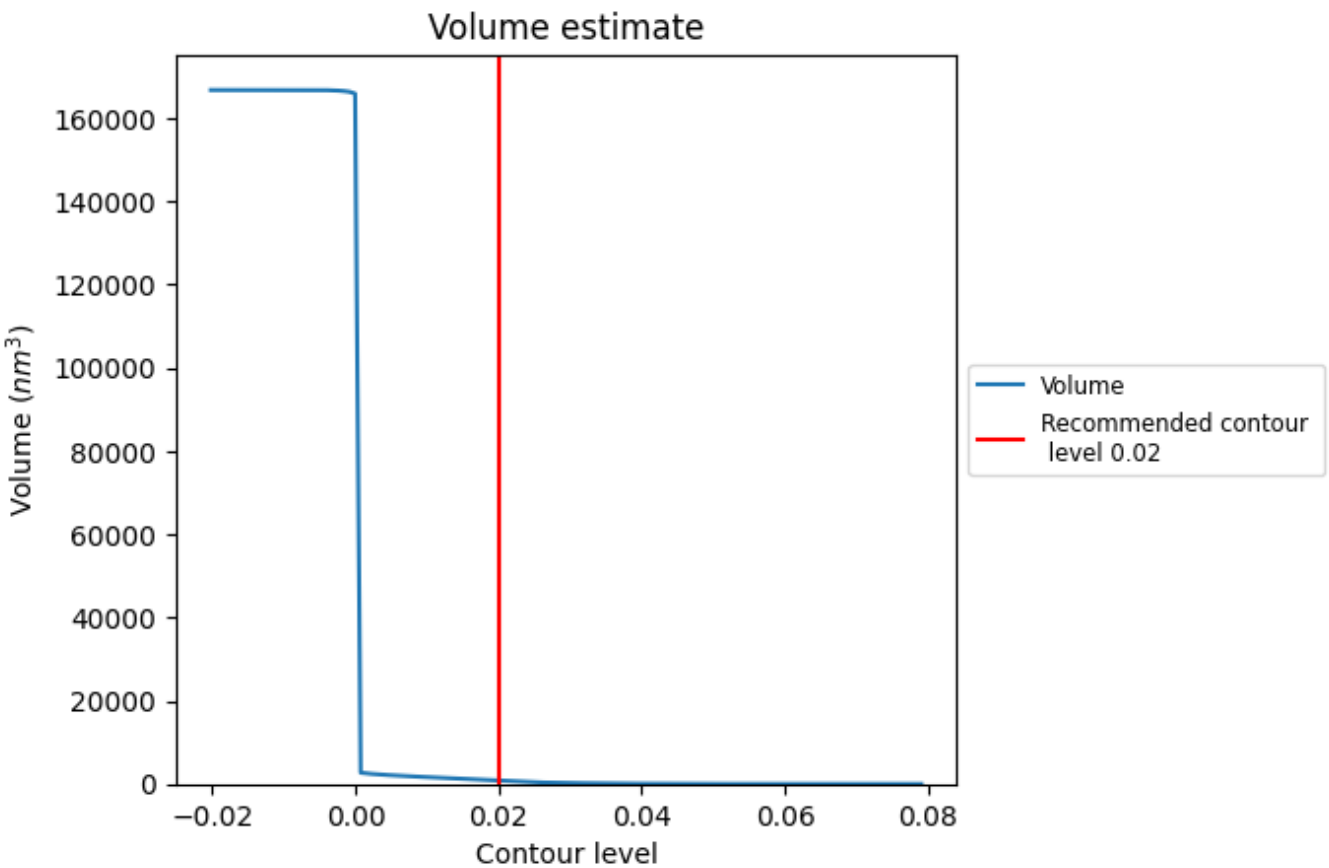
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

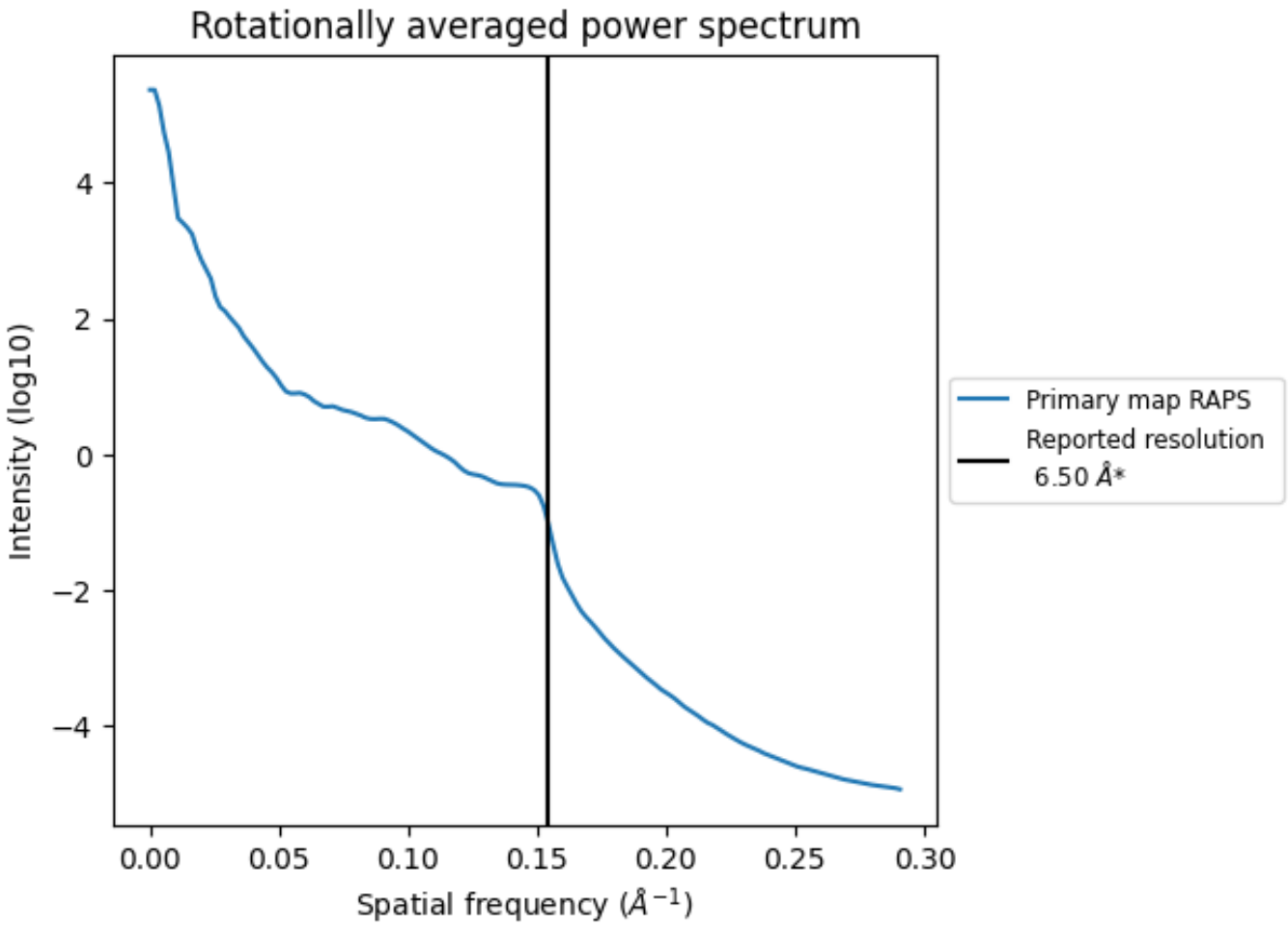
7.2 Volume estimate (i)



The volume at the recommended contour level is 787 nm^3; this corresponds to an approximate mass of 711 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 0.154 Å^{-1}

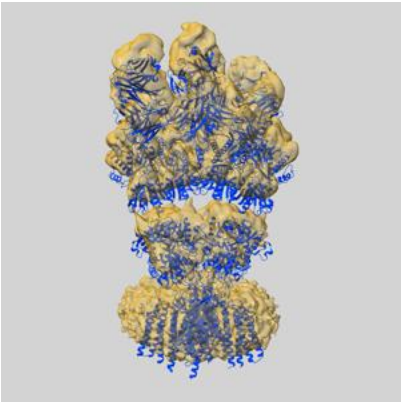
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

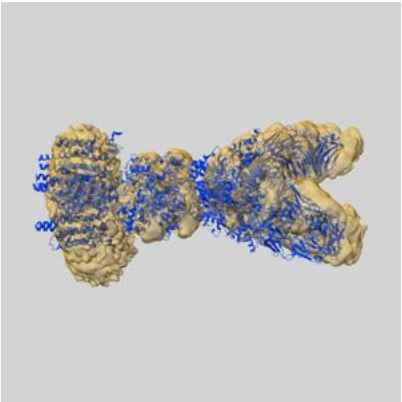
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9388 and PDB model 6NJM. Per-residue inclusion information can be found in section 3 on page 9.

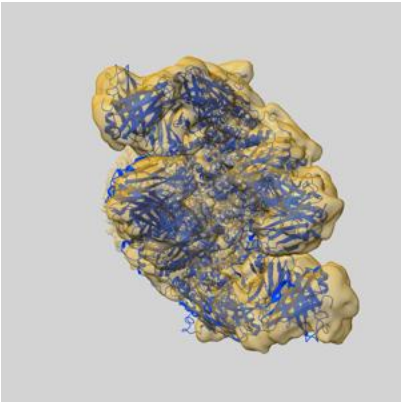
9.1 Map-model overlay (i)



X



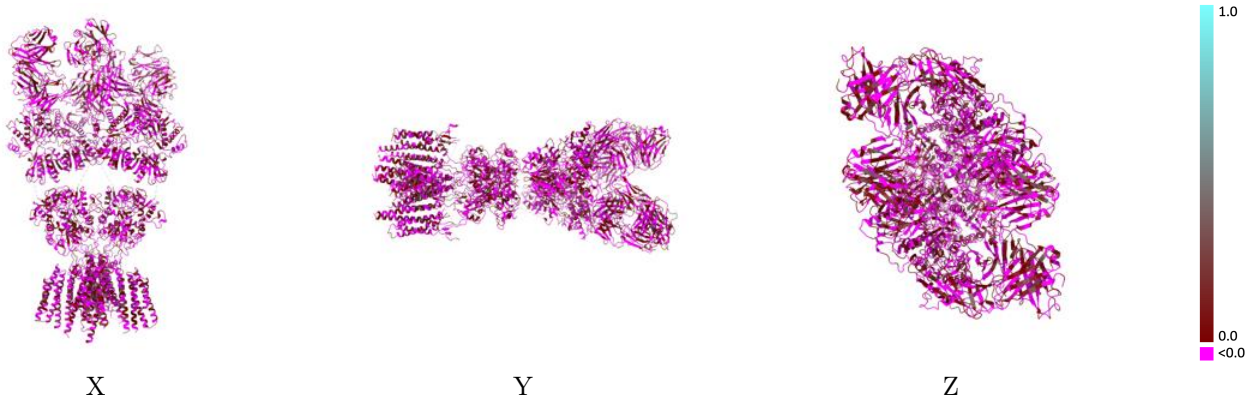
Y



Z

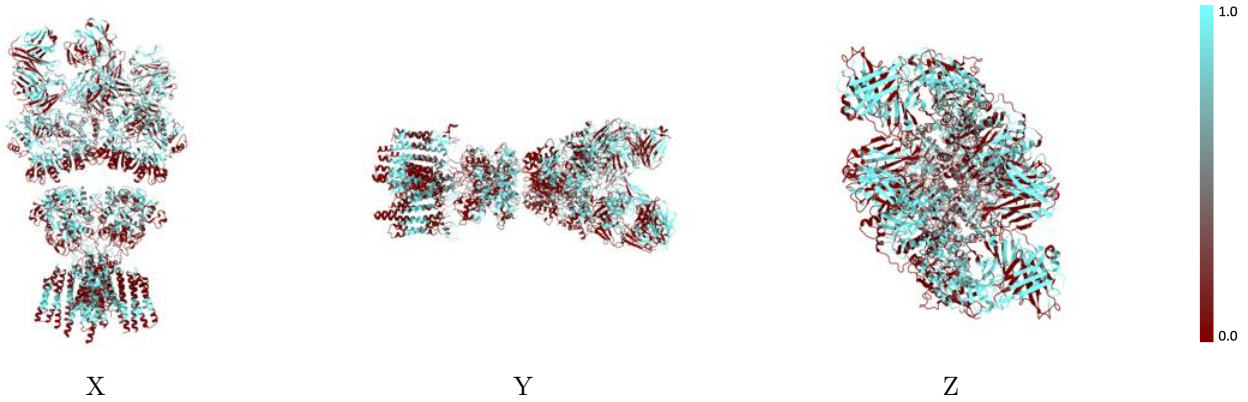
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



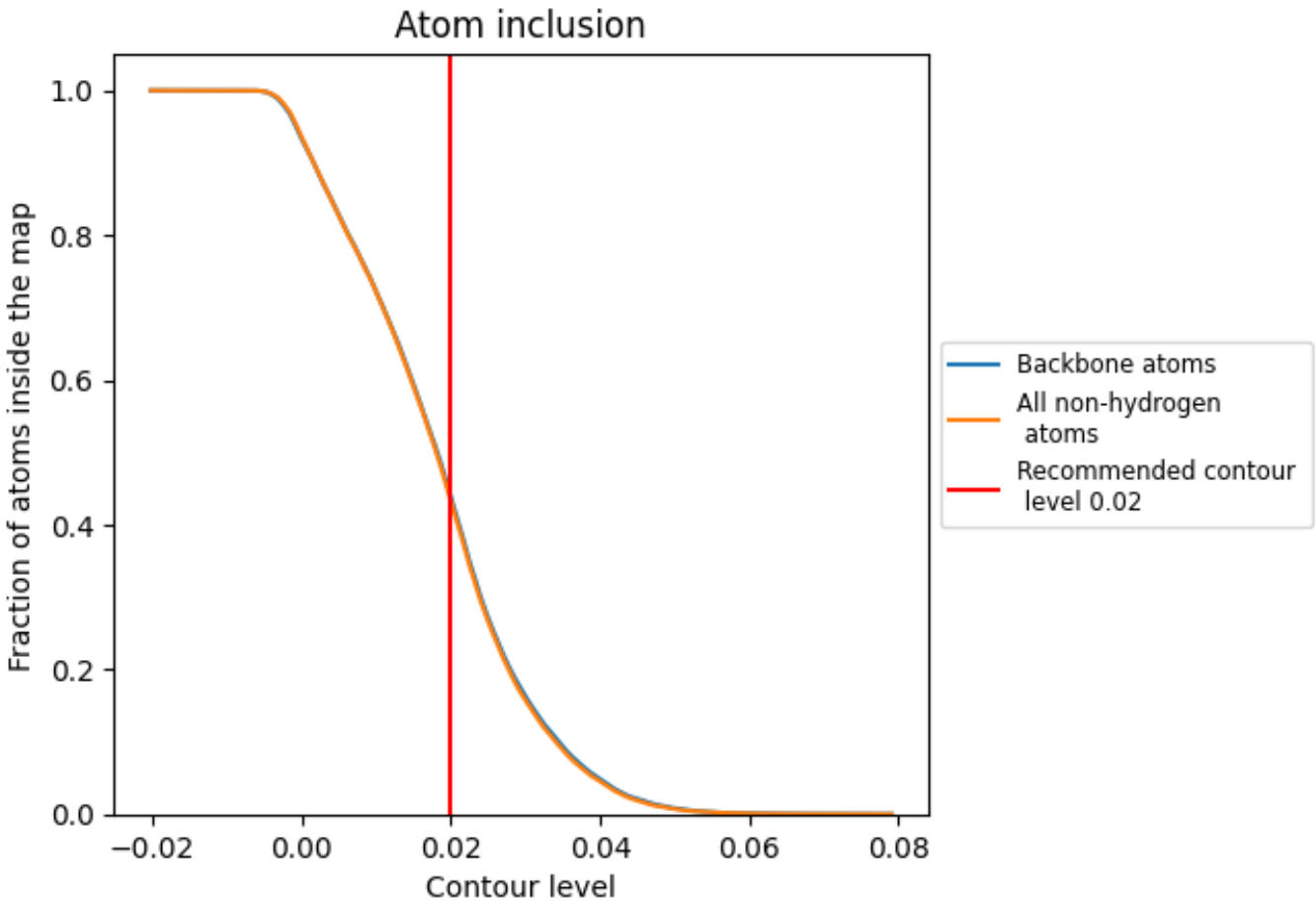
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 43% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4332	-0.0050
A	0.4428	-0.0070
B	0.4387	-0.0190
C	0.4115	0.0010
D	0.3903	-0.0030
E	0.3385	-0.0260
F	0.5115	0.0360
G	0.4291	-0.0200
H	0.4226	-0.0120
I	0.3119	-0.0280
J	0.6469	0.0230
K	0.5393	-0.0140
L	0.3059	-0.0320
M	0.4303	-0.0080
N	0.6329	0.0200
O	0.6180	0.0330
P	0.3173	-0.0090
Q	0.0000	-0.0360
R	0.1786	-0.0380
S	0.0000	-0.1150
T	0.1026	-0.0360
U	0.2143	-0.0240
V	0.0000	0.0640