Full wwPDB EM Validation Report ⓘ

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

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

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

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

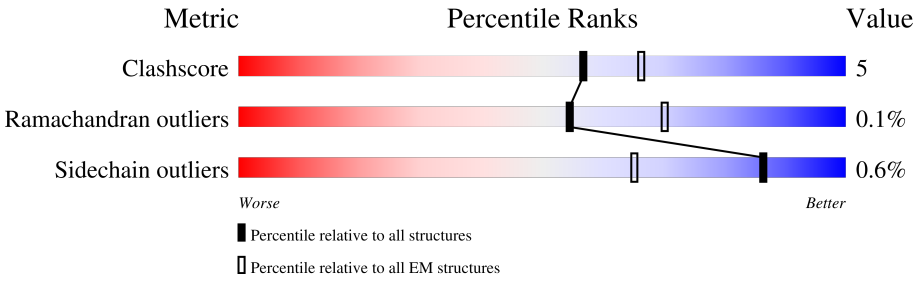
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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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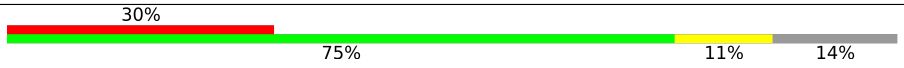
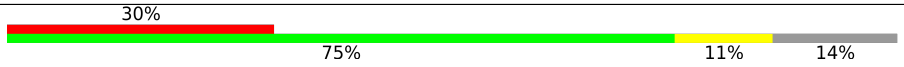
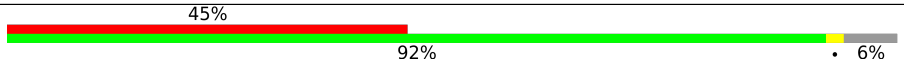
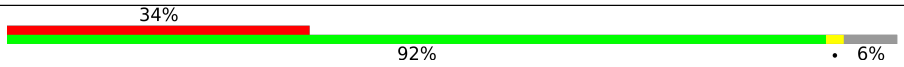
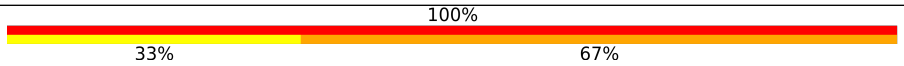
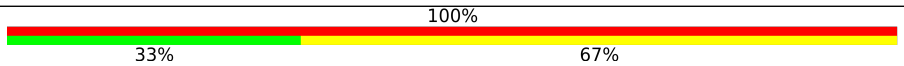
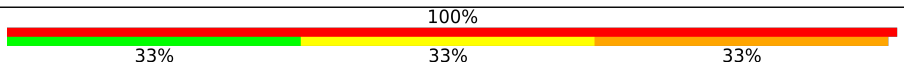
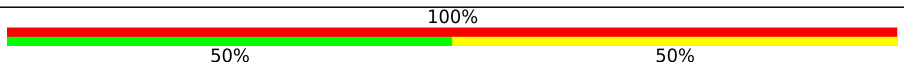
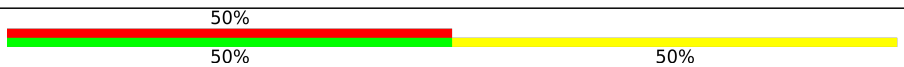
Mol	Chain	Length	Quality of chain
5	I	218	
5	M	218	
6	J	247	
6	N	247	
7	K	225	
7	O	225	
8	L	262	
8	P	262	
9	Q	3	
9	S	3	
9	T	3	
9	V	3	
10	R	2	
10	U	2	

2 Entry composition

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
1	A	784	Total	C	N	O	S	0	0
			6011	3866	995	1116	34		
1	C	784	Total	C	N	O	S	0	0
			6011	3866	995	1116	34		

- Molecule 2 is a protein called Glutamate receptor 2.

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

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
3	E	117	Total	C	N	O	0	0
			585	351	117	117		

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

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

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

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

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

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

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

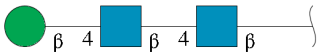
- Molecule 7 is a protein called 15F1 Fab light chain.

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

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

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

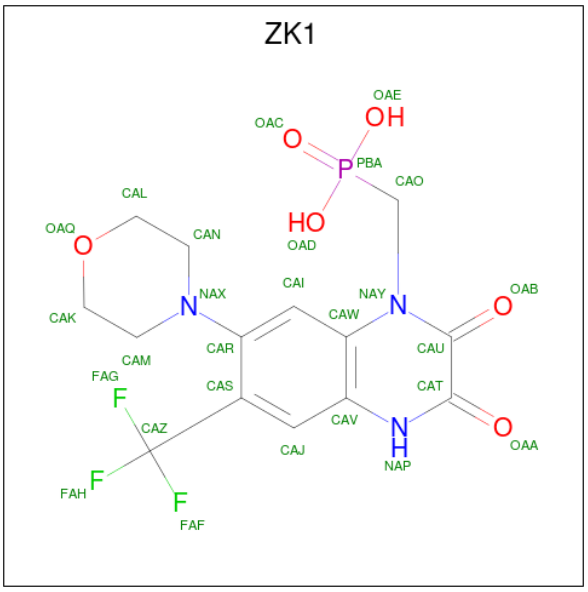


Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	3	Total	C	N	O	0	0
			39	22	2	15		
9	S	3	Total	C	N	O	0	0
			39	22	2	15		
9	T	3	Total	C	N	O	0	0
			39	22	2	15		
9	V	3	Total	C	N	O	0	0
			39	22	2	15		

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

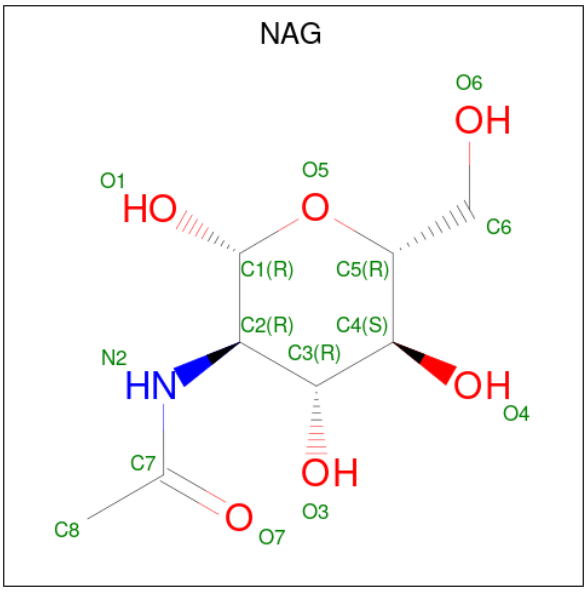
Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	2	Total	C	N	O	0	0
			28	16	2	10		
10	U	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
11	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
11	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
11	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
11	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

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



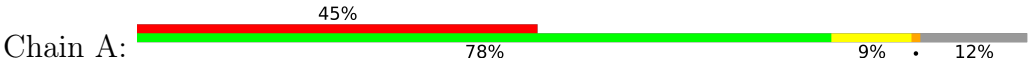
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	C	1	Total	C	N	O	0
			14	8	1	5	
12	D	1	Total	C	N	O	0
			14	8	1	5	

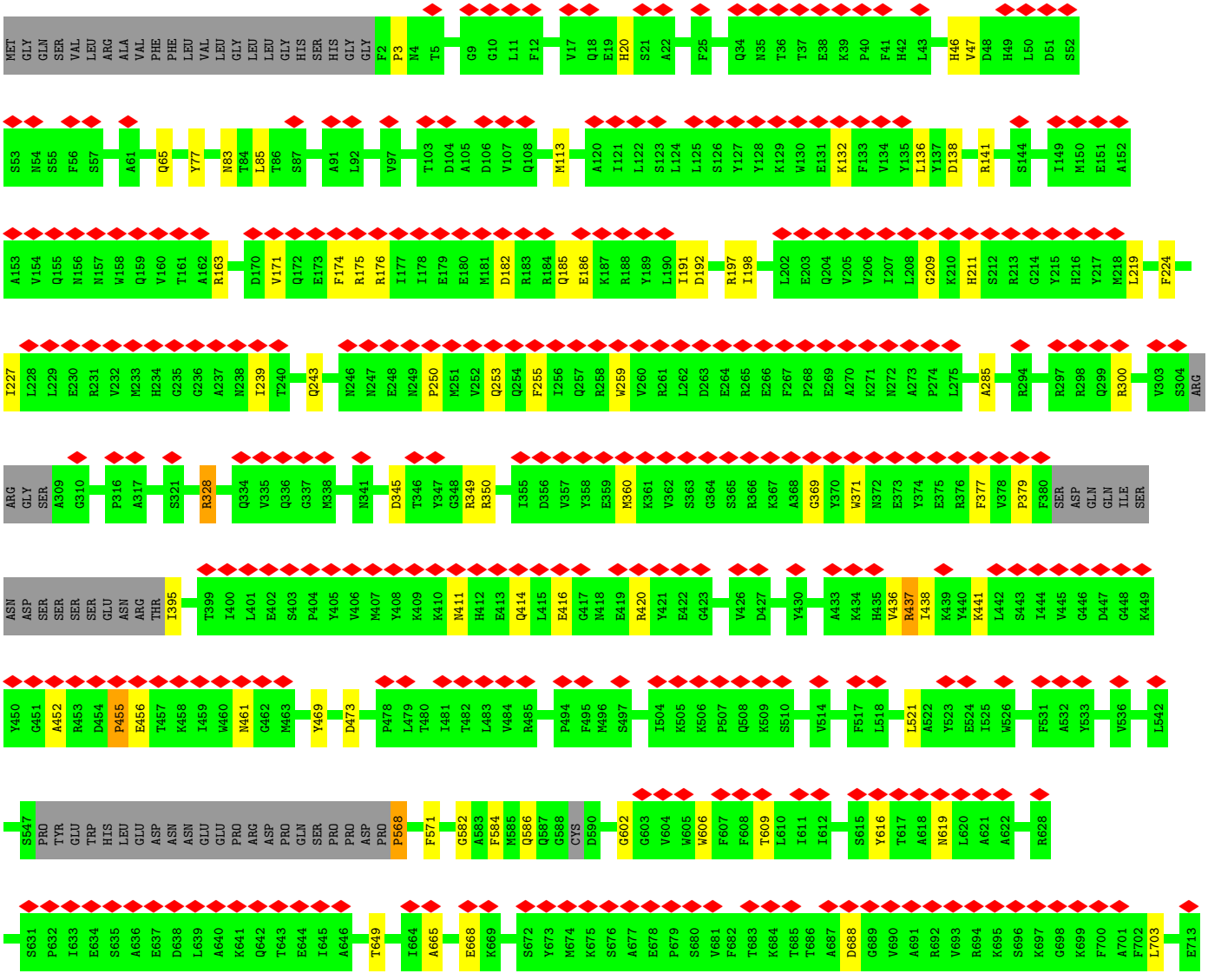
3 Residue-property plots (i)

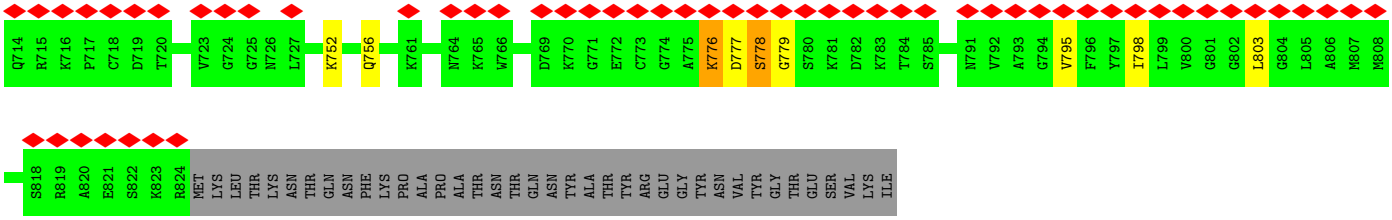
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor 3

Chain A:

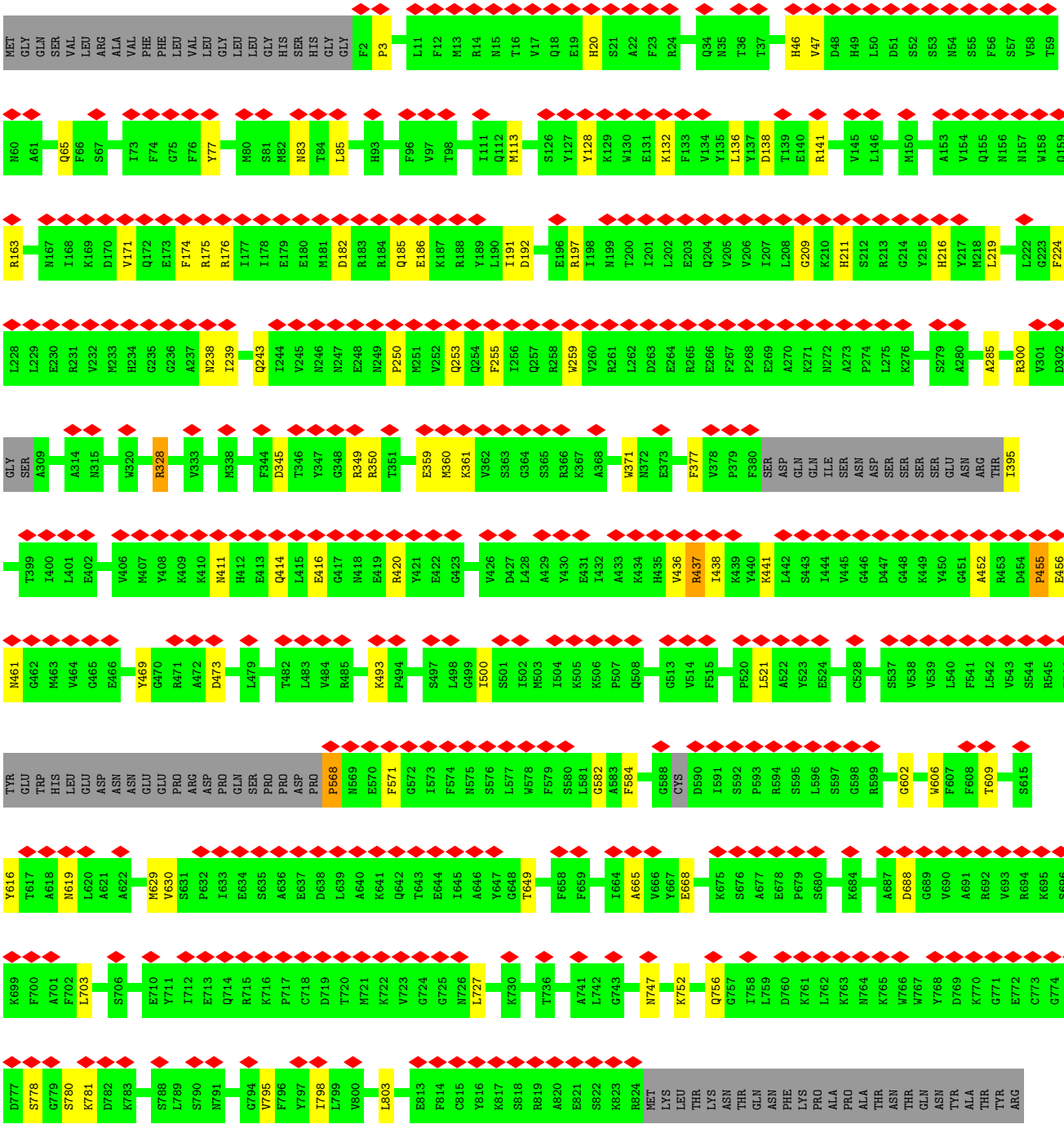






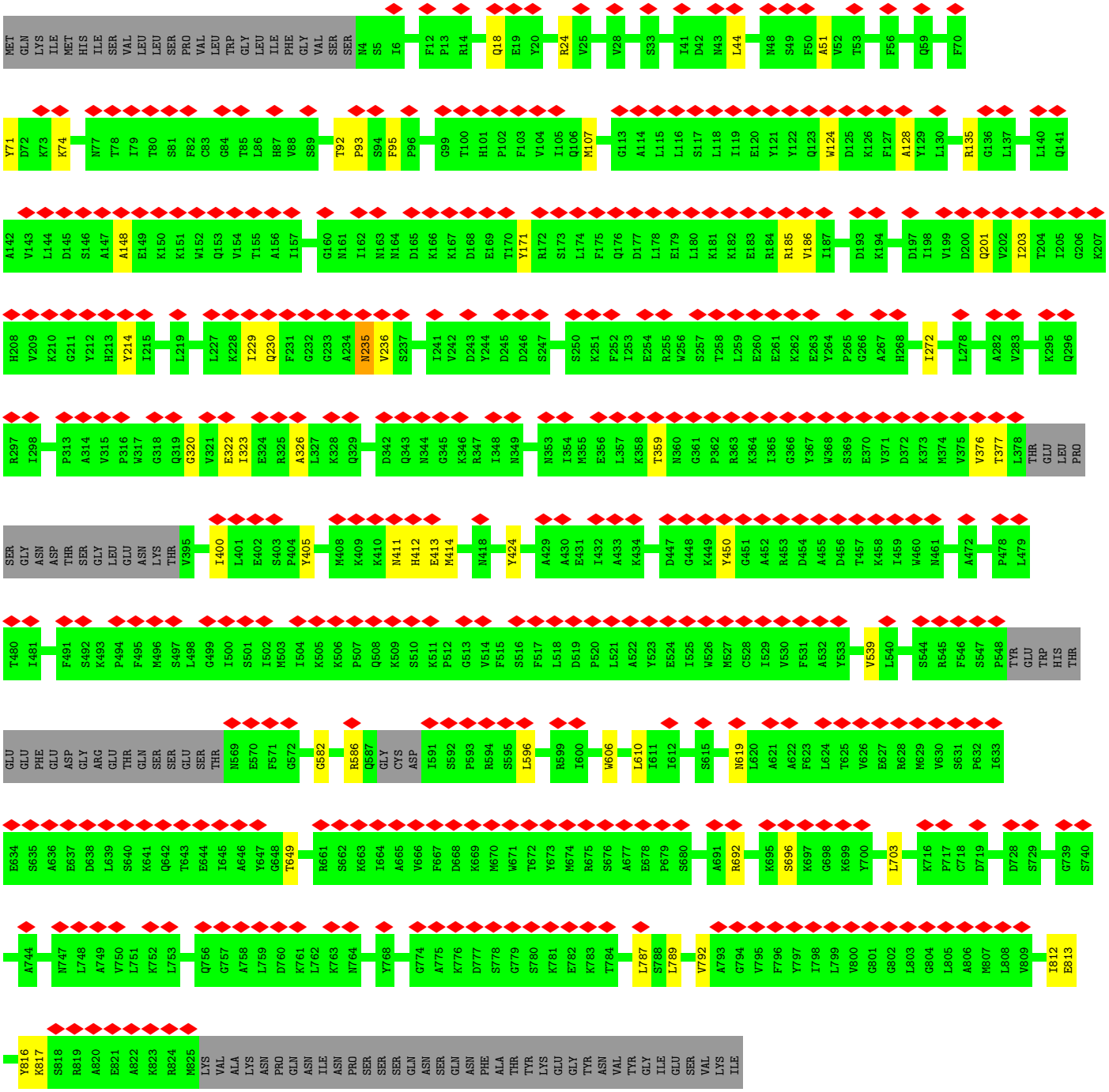
- Molecule 1: Glutamate receptor 3

Chain C:



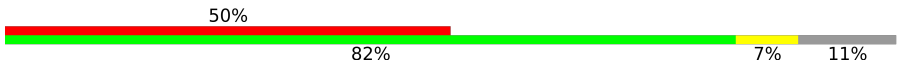
• Molecule 2: Glutamate receptor 2

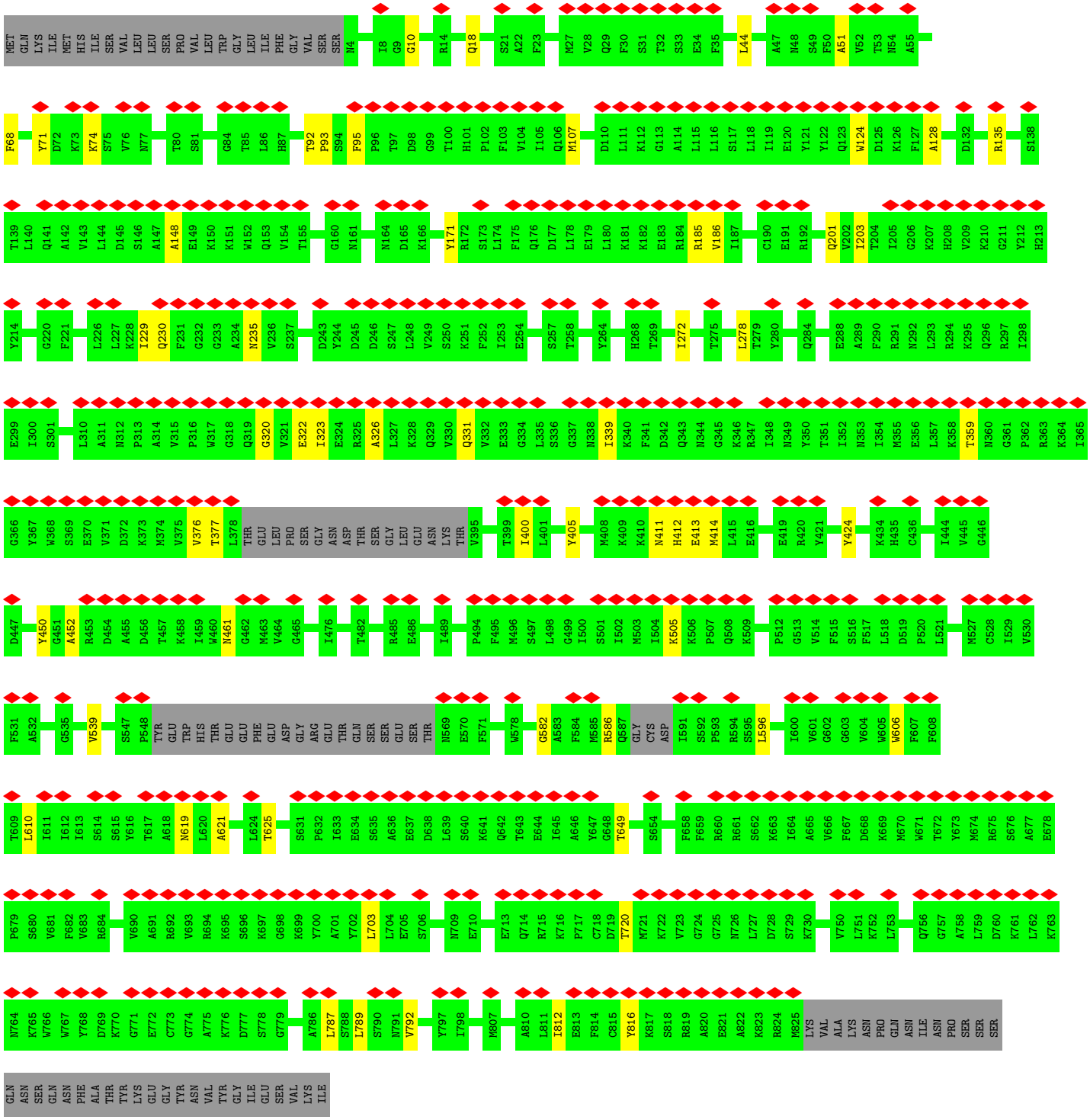
Chain B:



• Molecule 2: Glutamate receptor 2

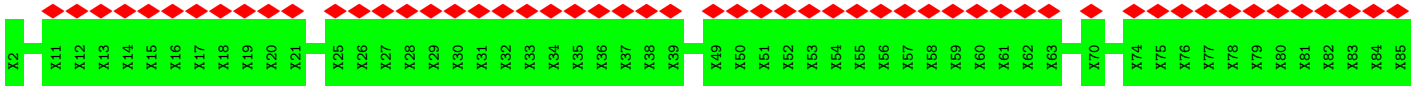
Chain D:

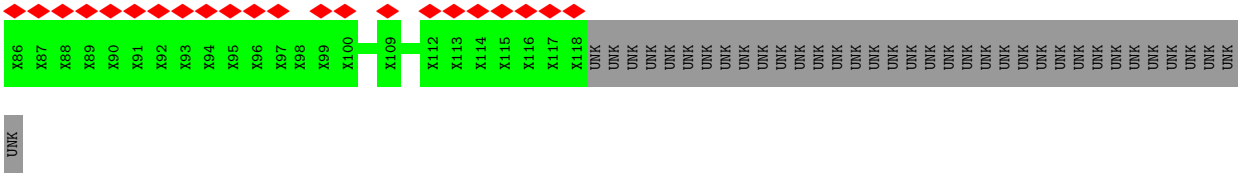




• Molecule 3: A'-C' auxiliary proteins

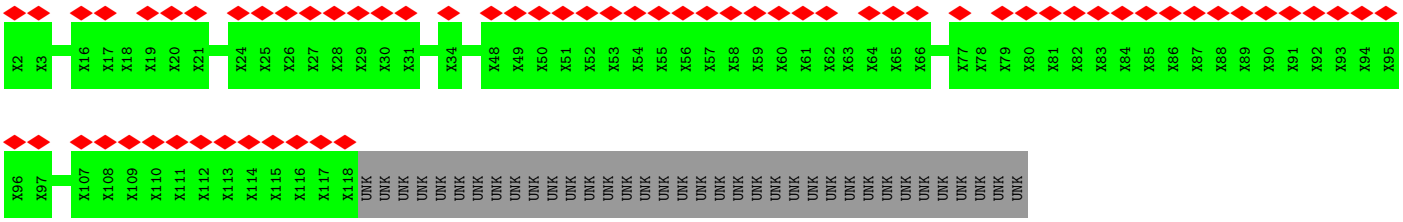
Chain E:





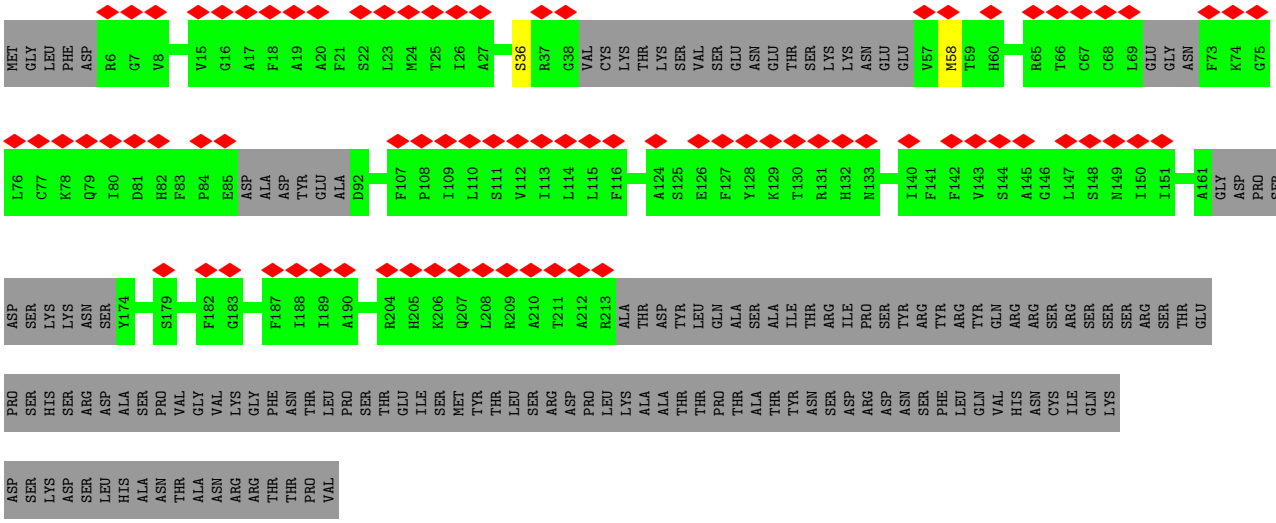
• Molecule 3: A'-C' auxiliary proteins

Chain G:



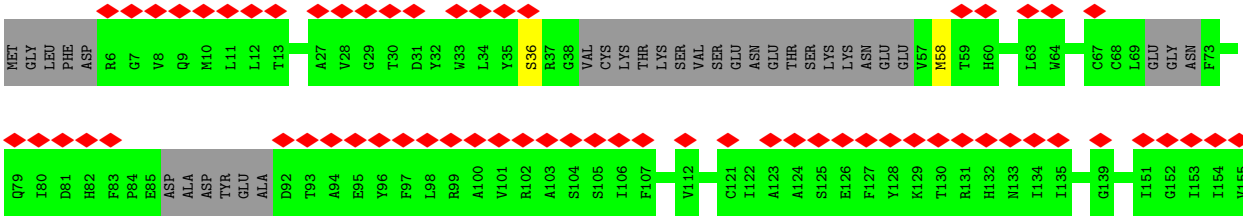
• Molecule 4: Voltage-dependent calcium channel gamma-2 subunit

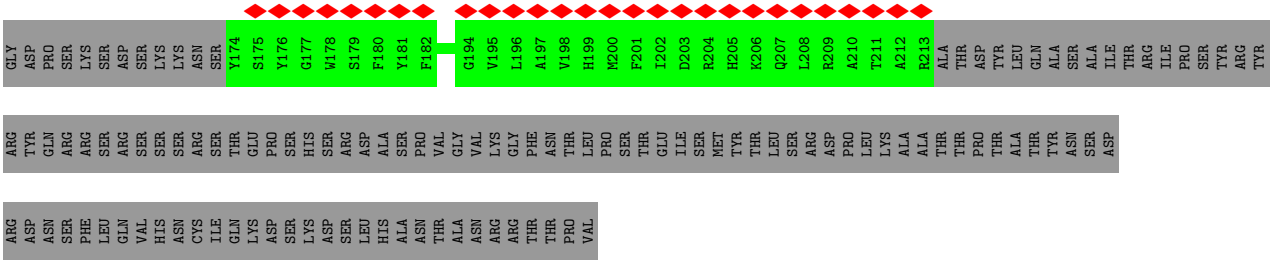
Chain F:



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

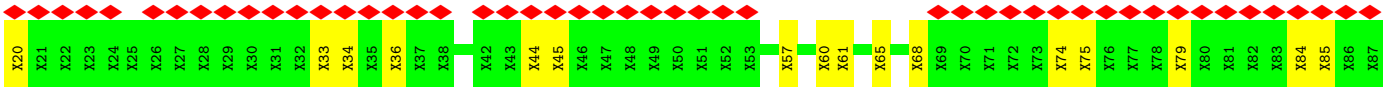
Chain H:

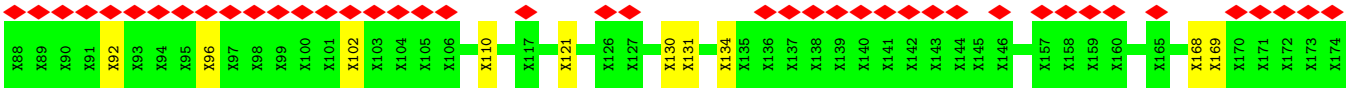


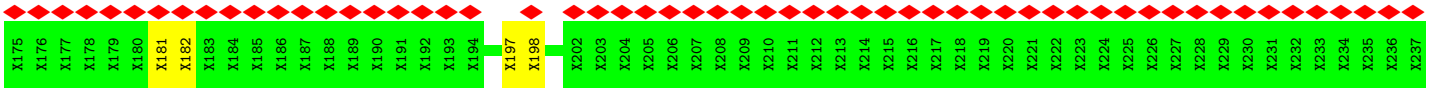


• Molecule 5: 5B2 Fab Light Chain

Chain I:

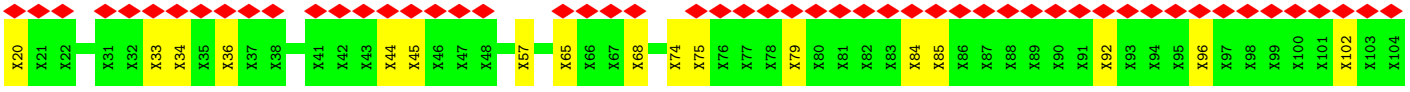


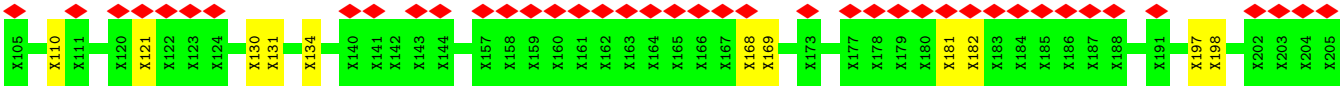


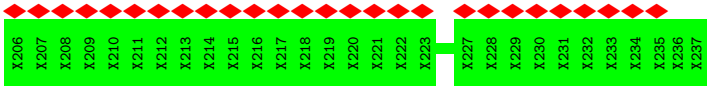


• Molecule 5: 5B2 Fab Light Chain

Chain M:

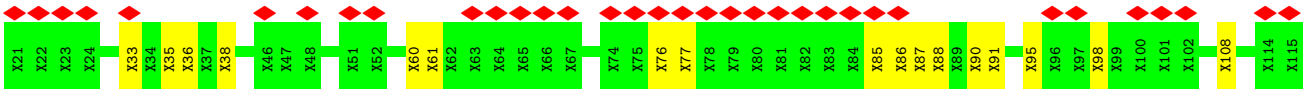


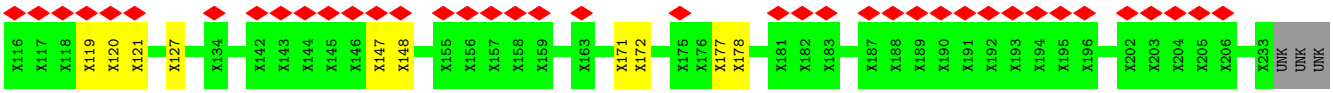




• Molecule 6: 5B2 Fab Heavy Chain

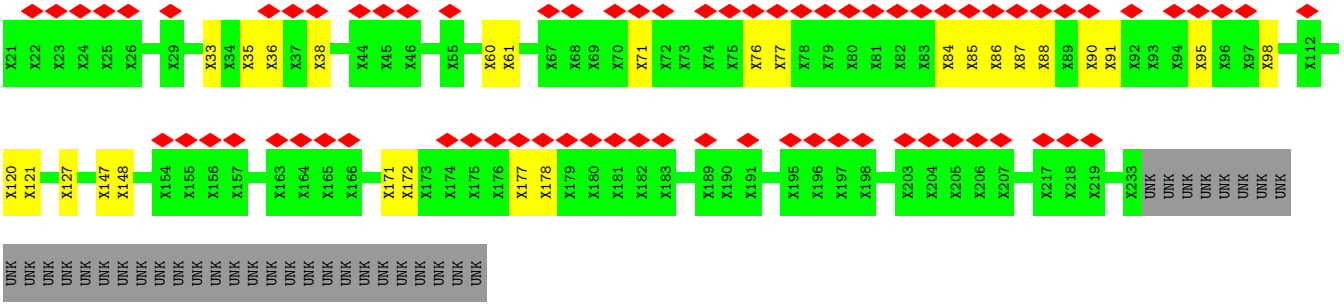
Chain J:





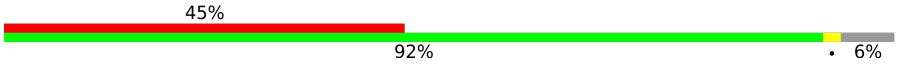
• Molecule 6: 5B2 Fab Heavy Chain

Chain N:



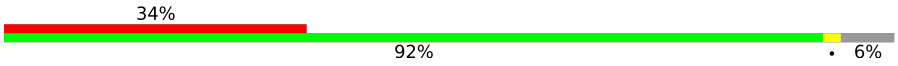
• Molecule 7: 15F1 Fab light chain

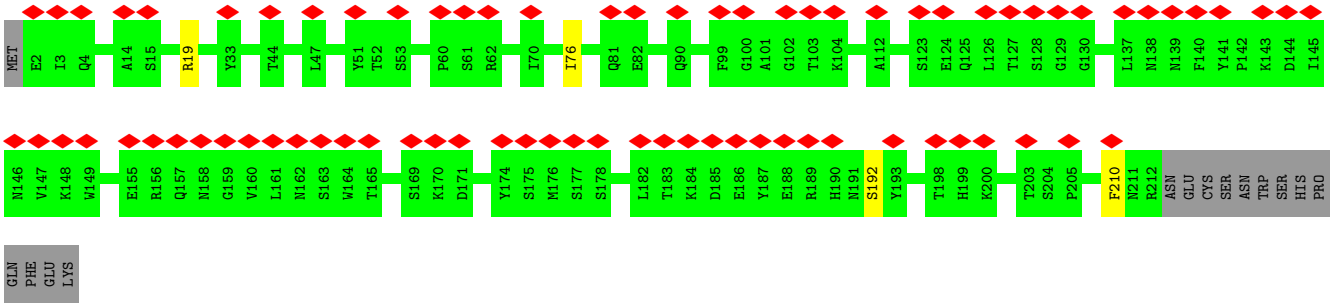
Chain K:



• Molecule 7: 15F1 Fab light chain

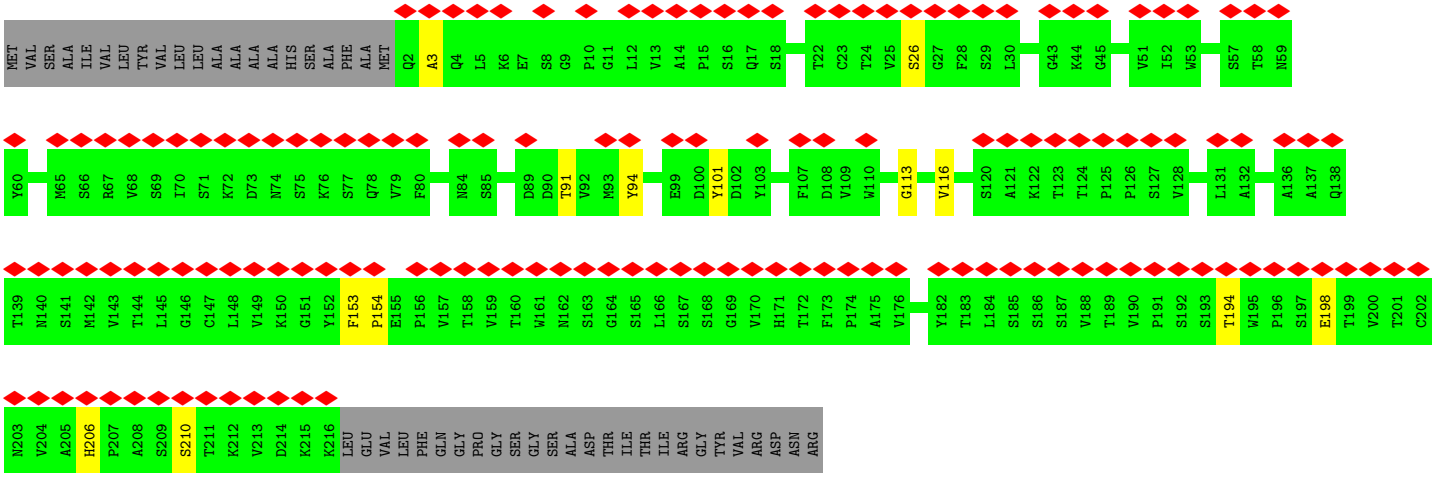
Chain O:





• Molecule 8: 15F1 Fab heavy chain

Chain L:

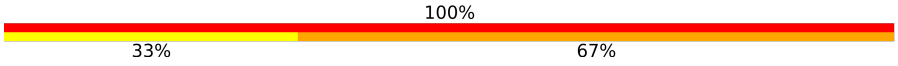


• Molecule 8: 15F1 Fab heavy chain

Chain P:

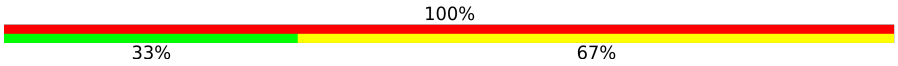
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

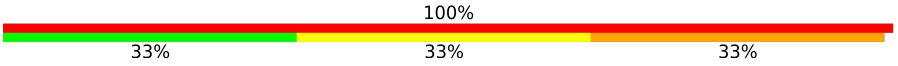


• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

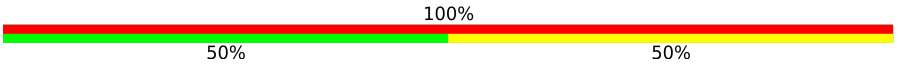
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

5.1 Standard geometry

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.

All (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
1	C	3	PRO	C-N-CA	6.57	138.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	596	LEU	CA-CB-CG	6.56	130.40	115.30
2	D	596	LEU	CA-CB-CG	6.53	130.31	115.30
1	C	688	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	688	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	473	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	473	ASP	CB-CG-OD2	5.16	122.95	118.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:A:185:GLN:CD	1:A:469:TYR:HE1	1.20	1.40
1:C:185:GLN:HG2	1:C:469:TYR:CE1	1.49	1.37
1:C:185:GLN:NE2	1:C:469:TYR:CE1	1.98	1.32
1:C:185:GLN:CG	1:C:469:TYR:HE1	1.29	1.30
1:A:777:ASP:O	1:A:779:GLY:N	1.65	1.28
5:I:20:UNK:O	5:I:45:UNK:CB	1.84	1.24
5:M:20:UNK:O	5:M:45:UNK:CB	1.85	1.22
1:A:185:GLN:HG2	1:A:469:TYR:CD1	1.76	1.20
1:C:185:GLN:HG2	1:C:469:TYR:CD1	1.77	1.19
1:A:185:GLN:NE2	1:A:469:TYR:CE1	2.10	1.19
1:A:185:GLN:CD	1:A:469:TYR:CE1	2.09	1.17
1:C:185:GLN:CG	1:C:469:TYR:CD1	2.33	1.12
6:J:86:UNK:CB	6:J:91:UNK:HA	1.81	1.11
1:C:185:GLN:CD	1:C:469:TYR:CE1	2.04	1.10
1:A:185:GLN:CG	1:A:469:TYR:CD1	2.33	1.09
6:N:86:UNK:CB	6:N:91:UNK:HA	1.82	1.07
2:B:812:ILE:O	2:B:816:TYR:HD2	1.39	1.03
2:D:812:ILE:O	2:D:816:TYR:HD2	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HD11	1:A:438:ILE:HG21	1.41	1.02
1:C:395:ILE:HD11	1:C:438:ILE:HG21	1.41	1.02
1:C:455:PRO:HD2	1:C:456:GLU:H	1.27	1.00
1:A:455:PRO:HD2	1:A:456:GLU:H	1.27	1.00
1:C:185:GLN:NE2	1:C:469:TYR:HE1	1.47	0.99
2:B:812:ILE:O	2:B:816:TYR:CD2	2.17	0.97
2:D:812:ILE:O	2:D:816:TYR:CD2	2.20	0.94
1:C:568:PRO:HD2	1:C:571:PHE:HB2	1.51	0.91
1:A:568:PRO:HD2	1:A:571:PHE:HB2	1.53	0.90
5:M:20:UNK:C	5:M:45:UNK:CB	2.51	0.89
1:A:185:GLN:HG3	1:A:469:TYR:CE1	2.06	0.88
1:C:395:ILE:HD12	1:C:438:ILE:HG22	1.54	0.87
1:C:395:ILE:CD1	1:C:438:ILE:CG2	2.52	0.87
7:O:19:ARG:HA	7:O:76:ILE:O	1.74	0.87
7:K:19:ARG:HA	7:K:76:ILE:O	1.74	0.87
1:C:395:ILE:HD11	1:C:438:ILE:CG2	2.06	0.85
1:C:395:ILE:CD1	1:C:438:ILE:HG21	2.06	0.85
2:D:376:VAL:HG12	2:D:377:THR:N	1.90	0.84
1:A:185:GLN:HG3	1:A:469:TYR:CD1	2.12	0.84
2:B:376:VAL:HG12	2:B:377:THR:N	1.90	0.84
1:A:395:ILE:HD12	1:A:438:ILE:HG22	1.60	0.84
5:I:20:UNK:C	5:I:45:UNK:CB	2.56	0.83
1:A:395:ILE:CD1	1:A:438:ILE:CG2	2.56	0.83
1:A:395:ILE:HD11	1:A:438:ILE:CG2	2.09	0.83
1:A:455:PRO:HD2	1:A:456:GLU:N	1.95	0.82
1:A:395:ILE:CD1	1:A:438:ILE:HG21	2.09	0.81
1:C:455:PRO:HD2	1:C:456:GLU:N	1.95	0.81
1:C:185:GLN:HG3	1:C:469:TYR:CD1	2.14	0.80
1:C:185:GLN:NE2	1:C:469:TYR:CZ	2.49	0.80
1:A:436:VAL:O	1:A:437:ARG:CB	2.30	0.79
6:N:38:UNK:HA	6:N:95:UNK:O	1.82	0.79
6:J:85:UNK:O	6:J:86:UNK:CB	2.29	0.79
5:M:110:UNK:HA	5:M:134:UNK:O	1.83	0.79
5:I:110:UNK:HA	5:I:134:UNK:O	1.83	0.79
1:C:436:VAL:O	1:C:437:ARG:CB	2.30	0.78
1:C:185:GLN:HG3	1:C:469:TYR:CE1	2.16	0.78
6:J:38:UNK:HA	6:J:95:UNK:O	1.82	0.78
1:C:568:PRO:CD	1:C:571:PHE:HB2	2.14	0.78
1:A:185:GLN:NE2	1:A:469:TYR:CZ	2.53	0.77
6:N:85:UNK:O	6:N:86:UNK:CB	2.30	0.77
1:A:568:PRO:CD	1:A:571:PHE:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:LYS:HE3	1:C:756:GLN:HE22	1.53	0.74
6:J:147:UNK:O	6:J:148:UNK:CB	2.34	0.74
6:N:147:UNK:O	6:N:148:UNK:CB	2.34	0.74
1:A:752:LYS:HE3	1:A:756:GLN:HE22	1.50	0.74
5:M:68:UNK:CB	5:M:79:UNK:HA	2.19	0.72
2:B:376:VAL:HG12	2:B:377:THR:H	1.55	0.72
6:N:86:UNK:CB	6:N:90:UNK:O	2.38	0.72
5:I:68:UNK:CB	5:I:79:UNK:HA	2.20	0.71
1:C:395:ILE:HD12	1:C:438:ILE:CG2	2.18	0.71
1:C:395:ILE:CD1	1:C:438:ILE:HG22	2.18	0.71
1:C:128:TYR:OH	1:C:359:GLU:OE2	2.06	0.71
2:B:376:VAL:CG1	2:B:377:THR:N	2.54	0.70
2:D:376:VAL:CG1	2:D:377:THR:N	2.54	0.70
6:N:76:UNK:O	6:N:77:UNK:CB	2.39	0.70
2:B:376:VAL:CG1	2:B:377:THR:H	2.05	0.69
6:J:86:UNK:CB	6:J:90:UNK:O	2.41	0.69
2:D:376:VAL:HG12	2:D:377:THR:H	1.56	0.69
1:C:752:LYS:HE3	1:C:756:GLN:NE2	2.08	0.68
2:D:376:VAL:CG1	2:D:377:THR:H	2.05	0.68
1:C:455:PRO:CD	1:C:456:GLU:H	2.05	0.68
1:A:752:LYS:HE3	1:A:756:GLN:NE2	2.08	0.68
1:C:113:MET:O	1:C:350:ARG:NH1	2.26	0.67
6:J:76:UNK:O	6:J:77:UNK:CB	2.43	0.67
1:A:395:ILE:HD12	1:A:438:ILE:CG2	2.23	0.66
6:J:87:UNK:O	6:J:88:UNK:CB	2.45	0.65
1:A:455:PRO:CD	1:A:456:GLU:H	2.05	0.65
5:I:130:UNK:O	5:I:131:UNK:CB	2.45	0.65
6:N:87:UNK:O	6:N:88:UNK:CB	2.44	0.65
6:J:35:UNK:O	6:J:36:UNK:CB	2.45	0.64
1:A:455:PRO:CD	1:A:456:GLU:N	2.62	0.63
1:A:416:GLU:HA	1:A:420:ARG:HE	1.63	0.63
2:B:323:ILE:O	2:B:326:ALA:HB3	1.99	0.63
6:N:35:UNK:O	6:N:36:UNK:CB	2.45	0.63
2:D:323:ILE:O	2:D:326:ALA:HB3	1.99	0.62
1:C:416:GLU:HA	1:C:420:ARG:HE	1.64	0.62
5:M:84:UNK:O	5:M:85:UNK:CB	2.48	0.62
1:A:395:ILE:CD1	1:A:438:ILE:HG22	2.22	0.62
5:I:84:UNK:O	5:I:85:UNK:CB	2.47	0.61
1:C:185:GLN:CG	1:C:469:TYR:HD1	2.12	0.61
5:M:130:UNK:O	5:M:131:UNK:CB	2.49	0.61
1:C:455:PRO:CD	1:C:456:GLU:N	2.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:HIS:CE1	2:D:413:GLU:HG3	2.37	0.60
1:C:185:GLN:HG3	1:C:469:TYR:HD1	1.66	0.59
6:J:120:UNK:O	6:J:121:UNK:CB	2.51	0.59
6:N:120:UNK:O	6:N:121:UNK:CB	2.49	0.58
2:B:812:ILE:HB	2:B:816:TYR:HE2	1.68	0.58
1:C:163:ARG:NH1	2:D:148:ALA:HB1	2.20	0.57
2:D:812:ILE:HB	2:D:816:TYR:HE2	1.70	0.57
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.86	0.57
5:M:33:UNK:O	5:M:34:UNK:CB	2.53	0.56
6:N:171:UNK:O	6:N:172:UNK:CB	2.54	0.56
2:B:93:PRO:HA	2:B:107:MET:HB2	1.88	0.56
1:A:182:ASP:OD2	1:A:211:HIS:NE2	2.27	0.56
2:D:93:PRO:HA	2:D:107:MET:HB2	1.88	0.56
1:A:163:ARG:NH1	2:B:148:ALA:HB1	2.20	0.56
1:C:239:ILE:HB	1:C:360:MET:HB2	1.87	0.56
1:A:300:ARG:NH2	5:I:121:UNK:O	2.39	0.56
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.86	0.56
5:I:33:UNK:O	5:I:34:UNK:CB	2.54	0.56
1:A:239:ILE:HB	1:A:360:MET:HB2	1.88	0.55
1:C:216:HIS:HA	1:C:238:ASN:HB2	1.87	0.55
6:J:171:UNK:O	6:J:172:UNK:CB	2.53	0.55
1:A:752:LYS:O	1:A:756:GLN:HG3	2.06	0.55
2:B:412:HIS:CE1	2:B:413:GLU:HG3	2.40	0.55
2:D:649:THR:HG22	2:D:703:LEU:HB2	1.88	0.55
8:P:91:THR:HA	8:P:116:VAL:O	2.06	0.55
1:C:300:ARG:NH2	5:M:121:UNK:O	2.39	0.55
1:C:752:LYS:O	1:C:756:GLN:HG3	2.05	0.55
1:C:209:GLY:O	1:C:211:HIS:ND1	2.40	0.55
1:A:777:ASP:O	1:A:778:SER:C	2.38	0.55
1:A:77:TYR:HB3	1:A:85:LEU:HD12	1.89	0.54
1:A:209:GLY:O	1:A:211:HIS:ND1	2.41	0.54
8:L:91:THR:HA	8:L:116:VAL:O	2.07	0.54
2:B:649:THR:HG22	2:B:703:LEU:HB2	1.88	0.54
1:C:77:TYR:HB3	1:C:85:LEU:HD12	1.89	0.53
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.74	0.53
5:M:44:UNK:O	5:M:45:UNK:CB	2.57	0.53
2:D:586:ARG:HH12	2:D:610:LEU:HD13	1.74	0.52
2:B:586:ARG:HH12	2:B:610:LEU:HD13	1.74	0.52
2:B:203:ILE:HD11	2:B:229:ILE:HG23	1.90	0.52
2:D:203:ILE:HD11	2:D:229:ILE:HG23	1.92	0.52
2:B:230:GLN:NE2	2:B:359:THR:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HA	1:C:174:PHE:HD2	1.75	0.51
6:N:177:UNK:O	6:N:178:UNK:CB	2.59	0.51
2:B:320:GLY:HA2	2:B:323:ILE:HD12	1.93	0.51
1:C:361:LYS:HZ1	10:U:1:NAG:H5	1.76	0.51
2:D:322:GLU:O	2:D:326:ALA:N	2.44	0.51
1:C:138:ASP:OD2	1:C:197:ARG:NH1	2.44	0.51
1:C:182:ASP:OD2	1:C:211:HIS:NE2	2.28	0.51
1:C:255:PHE:O	1:C:259:TRP:HB2	2.11	0.51
9:V:1:NAG:H83	9:V:2:NAG:H61	1.91	0.51
1:A:255:PHE:O	1:A:259:TRP:HB2	2.10	0.51
2:D:230:GLN:NE2	2:D:359:THR:O	2.42	0.51
5:M:181:UNK:O	5:M:182:UNK:CB	2.59	0.50
1:A:328:ARG:HH12	5:I:74:UNK:CB	2.25	0.50
2:B:235:ASN:OD1	2:B:235:ASN:N	2.45	0.50
1:C:361:LYS:NZ	10:U:1:NAG:H5	2.27	0.50
2:B:813:GLU:O	2:B:817:LYS:HG3	2.11	0.50
1:A:411:ASN:HB2	1:A:414:GLN:OE1	2.11	0.50
2:D:411:ASN:HB2	2:D:414:MET:HB2	1.94	0.49
2:B:322:GLU:O	2:B:326:ALA:N	2.44	0.49
1:A:171:VAL:HA	1:A:174:PHE:HD2	1.76	0.49
2:D:320:GLY:HA2	2:D:323:ILE:HD12	1.93	0.49
5:I:74:UNK:O	5:I:75:UNK:CB	2.60	0.49
6:J:60:UNK:O	6:J:61:UNK:CB	2.59	0.49
1:A:371:TRP:HA	1:A:377:PHE:HA	1.95	0.49
1:A:777:ASP:O	1:A:779:GLY:CA	2.56	0.49
1:A:803:LEU:HD11	2:D:539:VAL:HG21	1.95	0.49
6:N:60:UNK:O	6:N:61:UNK:CB	2.59	0.49
4:H:36:SER:HA	4:H:58:MET:HA	1.93	0.49
8:L:206:HIS:O	8:L:210:SER:N	2.46	0.48
1:C:345:ASP:OD1	1:C:349:ARG:N	2.44	0.48
2:D:171:TYR:HD2	2:D:201:GLN:HG3	1.78	0.48
1:C:606:TRP:HH2	2:D:582:GLY:HA2	1.78	0.48
1:A:345:ASP:OD1	1:A:349:ARG:N	2.42	0.48
1:A:582:GLY:HA2	2:D:606:TRP:HH2	1.77	0.48
6:J:177:UNK:O	6:J:178:UNK:CB	2.61	0.48
1:C:584:PHE:HA	1:C:609:THR:HG21	1.95	0.48
5:I:44:UNK:O	5:I:45:UNK:CB	2.60	0.48
1:A:752:LYS:CE	1:A:756:GLN:NE2	2.76	0.48
2:D:789:LEU:HD12	2:D:792:VAL:HB	1.96	0.48
8:P:206:HIS:O	8:P:210:SER:N	2.46	0.48
1:A:371:TRP:HD1	1:A:377:PHE:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:HIS:HD2	1:C:65:GLN:HE22	1.62	0.47
2:B:24:ARG:NE	8:L:101:TYR:O	2.46	0.47
1:C:752:LYS:CE	1:C:756:GLN:NE2	2.77	0.47
2:B:171:TYR:HD2	2:B:201:GLN:HG3	1.78	0.47
1:A:83:ASN:ND2	2:B:74:LYS:O	2.37	0.47
6:N:33:UNK:O	6:N:127:UNK:N	2.47	0.47
1:A:776:LYS:H	1:A:776:LYS:HD2	1.80	0.47
1:C:371:TRP:HA	1:C:377:PHE:HA	1.95	0.47
1:C:776:LYS:H	1:C:776:LYS:HD2	1.80	0.47
5:I:181:UNK:O	5:I:182:UNK:CB	2.62	0.47
1:C:20:HIS:HE1	1:C:47:VAL:HG21	1.79	0.47
1:A:20:HIS:HE1	1:A:47:VAL:HG21	1.79	0.47
6:J:33:UNK:O	6:J:127:UNK:N	2.48	0.47
2:B:411:ASN:HB2	2:B:414:MET:HB2	1.96	0.46
1:C:141:ARG:NH2	1:C:192:ASP:OD1	2.47	0.46
8:P:3:ALA:HA	8:P:26:SER:O	2.15	0.46
2:D:128:ALA:HB3	2:D:186:VAL:HG22	1.98	0.46
1:C:250:PRO:HA	1:C:253:GLN:HG2	1.98	0.46
1:A:521:LEU:HD22	2:B:787:LEU:HD22	1.98	0.46
1:A:584:PHE:HA	1:A:609:THR:HG21	1.97	0.46
1:A:602:GLY:O	1:A:606:TRP:HB2	2.16	0.46
2:B:124:TRP:CE2	2:B:185:ARG:HD3	2.51	0.46
2:D:124:TRP:CE2	2:D:185:ARG:HD3	2.51	0.46
5:M:197:UNK:O	5:M:198:UNK:CB	2.64	0.46
2:B:692:ARG:O	2:B:696:SER:OG	2.29	0.46
2:D:621:ALA:O	2:D:625:THR:OG1	2.32	0.46
1:A:46:HIS:HD2	1:A:65:GLN:HE22	1.62	0.45
1:A:141:ARG:NH2	1:A:192:ASP:OD1	2.45	0.45
1:A:250:PRO:HA	1:A:253:GLN:HG2	1.98	0.45
2:B:400:ILE:HG21	2:B:450:TYR:HE1	1.82	0.45
1:A:185:GLN:HG3	1:A:469:TYR:HD1	1.70	0.45
1:C:411:ASN:HB2	1:C:414:GLN:OE1	2.17	0.45
2:D:400:ILE:HG21	2:D:450:TYR:HE1	1.81	0.45
1:C:132:LYS:HE2	1:C:186:GLU:OE2	2.17	0.45
1:C:224:PHE:HD2	1:C:243:GLN:HE21	1.64	0.45
1:C:395:ILE:O	1:C:441:LYS:N	2.50	0.45
4:F:36:SER:HA	4:F:58:MET:HA	1.98	0.45
8:L:153:PHE:HA	8:L:154:PRO:HA	1.84	0.45
1:A:369:GLY:HA3	1:A:379:PRO:HA	1.98	0.45
1:C:452:ALA:N	1:C:461:ASN:OD1	2.50	0.45
1:A:395:ILE:O	1:A:441:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LEU:HD21	1:A:616:TYR:HA	1.99	0.44
2:B:405:TYR:HA	2:B:424:TYR:HB3	1.99	0.44
1:C:780:SER:OG	1:C:781:LYS:N	2.50	0.44
11:A:901:ZK1:HAI	11:A:901:ZK1:HAOA	1.78	0.44
2:D:405:TYR:HA	2:D:424:TYR:HB3	1.98	0.44
5:M:74:UNK:O	5:M:75:UNK:CB	2.64	0.44
1:C:136:LEU:HD12	1:C:191:ILE:HG12	1.99	0.44
1:A:136:LEU:HD12	1:A:191:ILE:HG12	2.00	0.44
1:A:606:TRP:HH2	2:B:582:GLY:HA2	1.82	0.44
1:A:795:VAL:HA	1:A:798:ILE:HG22	2.00	0.44
1:C:219:LEU:HD13	1:C:227:ILE:HD13	2.00	0.44
1:C:328:ARG:HH12	5:M:74:UNK:CB	2.31	0.44
6:N:36:UNK:N	6:N:98:UNK:O	2.51	0.44
1:A:219:LEU:HD13	1:A:227:ILE:HD13	1.99	0.44
1:C:371:TRP:HD1	1:C:377:PHE:HB2	1.82	0.44
6:J:36:UNK:N	6:J:98:UNK:O	2.51	0.44
9:Q:1:NAG:H4	9:Q:2:NAG:H2	1.72	0.44
6:N:71:UNK:O	6:N:84:UNK:CB	2.66	0.44
1:C:602:GLY:O	1:C:606:TRP:HB2	2.17	0.43
2:D:44:LEU:HD23	2:D:51:ALA:HB1	2.00	0.43
9:Q:2:NAG:H4	9:Q:3:BMA:H2	1.89	0.43
2:B:606:TRP:HH2	1:C:582:GLY:HA2	1.84	0.43
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.99	0.43
1:C:795:VAL:HA	1:C:798:ILE:HG22	2.00	0.43
1:A:224:PHE:HD2	1:A:243:GLN:HE21	1.66	0.43
2:B:789:LEU:HD12	2:B:792:VAL:HB	2.00	0.43
1:A:185:GLN:NE2	1:A:469:TYR:OH	2.51	0.43
5:I:57:UNK:O	5:I:65:UNK:N	2.52	0.43
5:I:197:UNK:O	5:I:198:UNK:CB	2.65	0.43
1:A:452:ALA:N	1:A:461:ASN:OD1	2.50	0.43
8:P:206:HIS:O	8:P:210:SER:HA	2.18	0.43
1:A:132:LYS:HE2	1:A:186:GLU:OE2	2.19	0.43
2:B:71:TYR:OH	2:B:95:PHE:O	2.32	0.43
1:C:521:LEU:HD21	1:C:616:TYR:HA	2.01	0.43
1:C:602:GLY:O	1:C:606:TRP:CB	2.67	0.43
8:L:206:HIS:O	8:L:210:SER:CA	2.67	0.43
1:A:138:ASP:OD2	1:A:197:ARG:NH1	2.52	0.43
8:L:194:THR:O	8:L:198:GLU:N	2.47	0.43
2:B:44:LEU:HD23	2:B:51:ALA:HB1	2.00	0.42
1:C:83:ASN:ND2	2:D:74:LYS:O	2.37	0.42
1:C:521:LEU:HD22	2:D:787:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:901:ZK1:HAOA	11:D:901:ZK1:HAI	1.78	0.42
1:A:113:MET:HG3	1:A:285:ALA:HB2	2.01	0.42
8:L:206:HIS:O	8:L:210:SER:HA	2.18	0.42
8:P:153:PHE:HA	8:P:154:PRO:HA	1.84	0.42
8:P:206:HIS:O	8:P:210:SER:CA	2.67	0.42
1:A:113:MET:O	1:A:350:ARG:NH1	2.45	0.42
5:I:36:UNK:HA	5:I:102:UNK:O	2.19	0.42
8:P:94:TYR:O	8:P:113:GLY:HA2	2.19	0.42
5:I:60:UNK:O	5:I:61:UNK:CB	2.67	0.42
5:I:92:UNK:O	5:I:96:UNK:N	2.53	0.42
1:A:665:ALA:HA	1:A:668:GLU:HB2	2.02	0.42
1:A:171:VAL:HG23	1:A:175:ARG:NH1	2.35	0.41
8:L:94:TYR:O	8:L:113:GLY:HA2	2.20	0.41
1:C:113:MET:HG3	1:C:285:ALA:HB2	2.01	0.41
1:C:629:MET:HB3	1:C:630:VAL:H	1.70	0.41
1:C:665:ALA:HA	1:C:668:GLU:HB2	2.02	0.41
2:D:452:ALA:N	2:D:461:ASN:OD1	2.52	0.41
2:B:128:ALA:HB3	2:B:186:VAL:HG22	2.02	0.41
7:O:192:SER:HA	7:O:210:PHE:O	2.21	0.41
1:A:586:GLN:HB3	2:B:586:ARG:HG2	2.01	0.41
2:B:539:VAL:HG21	1:C:803:LEU:HD11	2.01	0.41
2:D:18:GLN:HE21	2:D:272:ILE:HG13	1.85	0.41
2:D:71:TYR:OH	2:D:95:PHE:O	2.32	0.41
1:A:602:GLY:O	1:A:606:TRP:CB	2.68	0.41
1:C:185:GLN:NE2	1:C:469:TYR:OH	2.54	0.41
2:D:107:MET:HB3	2:D:278:LEU:HD22	2.03	0.41
2:D:505:LYS:HA	2:D:720:THR:HA	2.03	0.41
5:M:36:UNK:HA	5:M:102:UNK:O	2.21	0.41
5:M:57:UNK:O	5:M:65:UNK:N	2.53	0.41
5:M:92:UNK:O	5:M:96:UNK:N	2.54	0.41
2:B:214:TYR:HB2	2:B:236:VAL:HG22	2.03	0.41
2:D:10:GLY:HA2	2:D:68:PHE:O	2.20	0.41
2:D:71:TYR:HE1	2:D:92:THR:HG21	1.85	0.41
2:D:331:GLN:HA	2:D:339:ILE:O	2.21	0.41
6:J:108:UNK:O	6:J:119:UNK:N	2.54	0.41
8:L:3:ALA:HA	8:L:26:SER:O	2.20	0.41
1:A:777:ASP:C	1:A:779:GLY:H	2.11	0.40
1:C:171:VAL:HG23	1:C:175:ARG:HH12	1.87	0.40
5:M:168:UNK:O	5:M:169:UNK:CB	2.69	0.40
2:B:18:GLN:HE21	2:B:272:ILE:HG13	1.86	0.40
5:I:168:UNK:O	5:I:169:UNK:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:TYR:HE1	2:B:92:THR:HG21	1.85	0.40
1:C:171:VAL:HG23	1:C:175:ARG:NH1	2.36	0.40
11:B:901:ZK1:HAI	11:B:901:ZK1:HAOA	1.77	0.40
1:C:452:ALA:O	1:C:460:TRP:HA	2.22	0.40
7:K:192:SER:HA	7:K:210:PHE:O	2.21	0.40
8:P:195:TRP:HA	8:P:196:PRO:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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
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

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Mol	Chain	Res	Type
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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	198	ILE
1	A	328	ARG
1	A	619	ASN
1	A	776	LYS
2	B	135	ARG
2	B	235	ASN
2	B	619	ASN
1	C	176	ARG
1	C	328	ARG
1	C	619	ASN
1	C	776	LYS
2	D	135	ARG
2	D	619	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	46	HIS
1	A	112	GLN
1	A	185	GLN
1	A	756	GLN
2	B	18	GLN
2	B	240	GLN
2	B	619	ASN
1	C	20	HIS
1	C	46	HIS
1	C	112	GLN
1	C	185	GLN
1	C	343	GLN
1	C	756	GLN
2	D	18	GLN
2	D	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

All (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
9	V	2	NAG	C1-C2	2.11	1.55	1.52

All (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
9	Q	1	NAG	C1-C2-N2	3.77	116.94	110.49
9	V	2	NAG	C4-C3-C2	3.43	116.04	111.02
9	S	1	NAG	C1-C2-N2	3.33	116.18	110.49
9	V	2	NAG	C2-N2-C7	3.02	127.21	122.90
10	R	2	NAG	C2-N2-C7	3.01	127.19	122.90
9	S	2	NAG	C1-O5-C5	2.55	115.64	112.19
9	T	1	NAG	C3-C4-C5	2.52	114.73	110.24
9	Q	3	BMA	C1-O5-C5	2.30	115.31	112.19
9	S	1	NAG	C8-C7-N2	2.29	119.98	116.10
9	T	1	NAG	C8-C7-N2	2.13	119.70	116.10
9	Q	1	NAG	C8-C7-N2	2.13	119.70	116.10
9	T	1	NAG	O4-C4-C3	-2.13	105.44	110.35
9	Q	1	NAG	C3-C4-C5	2.04	113.88	110.24
9	V	2	NAG	C1-C2-N2	2.03	113.96	110.49

There are no chirality outliers.

All (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
9	S	1	NAG	C8-C7-N2-C2
9	S	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	T	1	NAG	C8-C7-N2-C2
9	T	1	NAG	O7-C7-N2-C2
10	U	1	NAG	C8-C7-N2-C2
10	U	1	NAG	O7-C7-N2-C2
9	Q	2	NAG	O5-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
10	U	2	NAG	O5-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
9	T	1	NAG	C4-C5-C6-O6
9	S	1	NAG	C4-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	T	2	NAG	C4-C5-C6-O6
9	S	1	NAG	C3-C2-N2-C7
9	T	1	NAG	C3-C2-N2-C7
9	Q	1	NAG	C3-C2-N2-C7
9	V	2	NAG	C3-C2-N2-C7
10	R	2	NAG	C3-C2-N2-C7

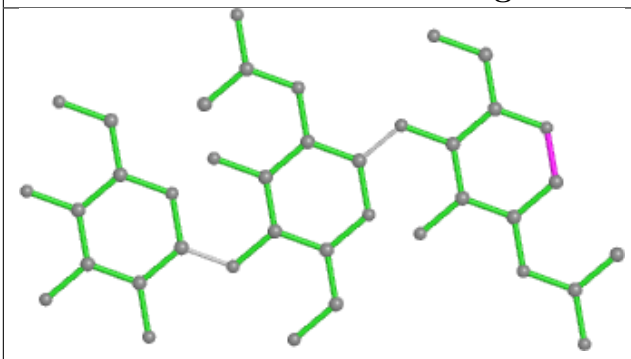
There are no ring outliers.

6 monomers are involved in 5 short contacts:

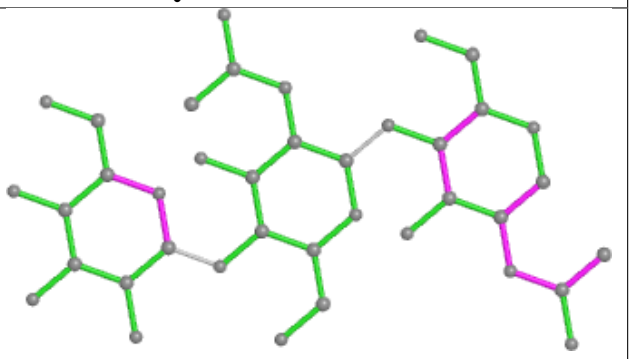
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	2	NAG	2	0
9	Q	1	NAG	1	0
10	U	1	NAG	2	0
9	Q	3	BMA	1	0
9	V	1	NAG	1	0
9	V	2	NAG	1	0

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

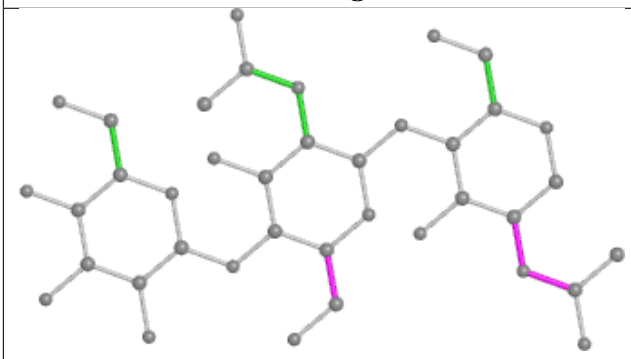
Oligosaccharide Chain Q



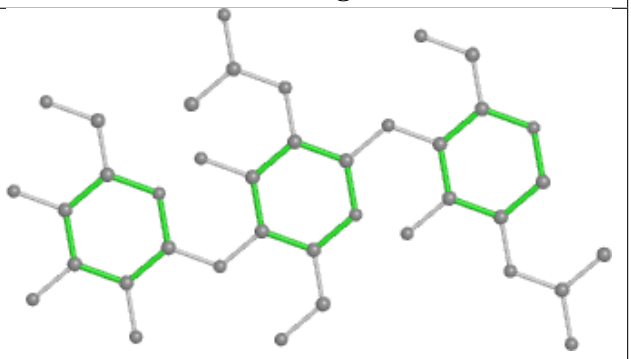
Bond lengths



Bond angles

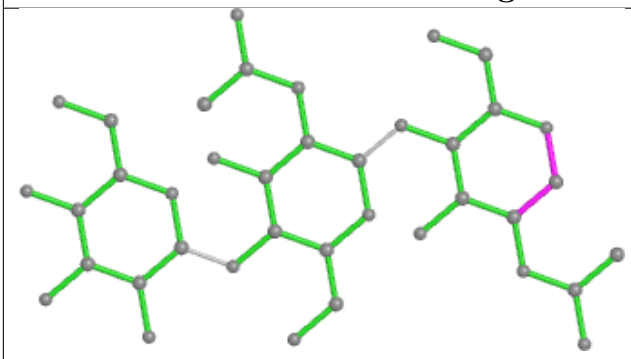


Torsions

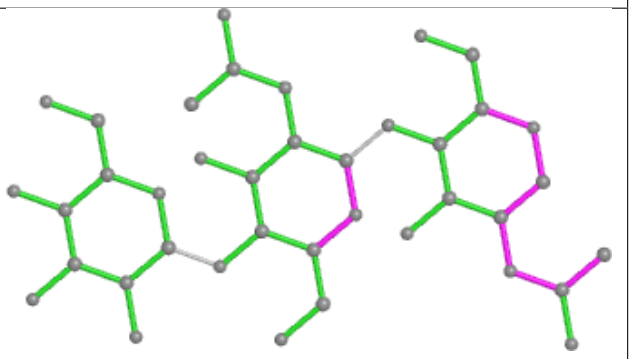


Rings

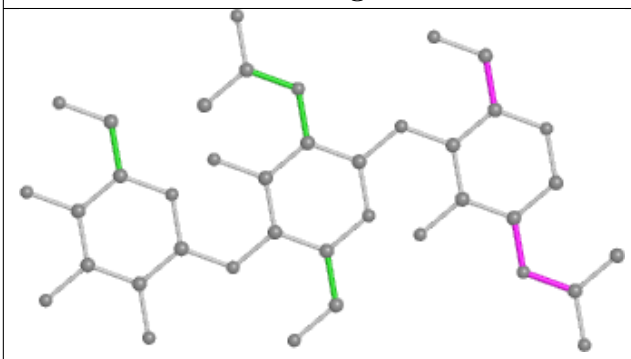
Oligosaccharide Chain S



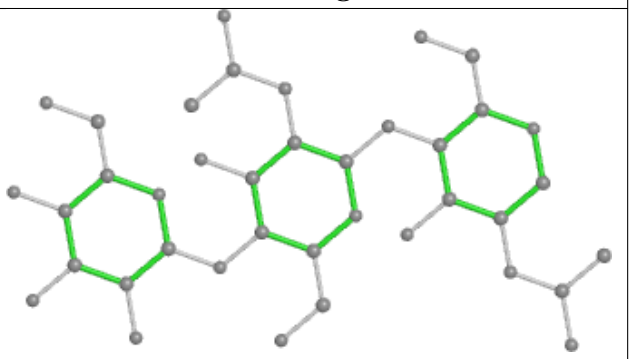
Bond lengths



Bond angles

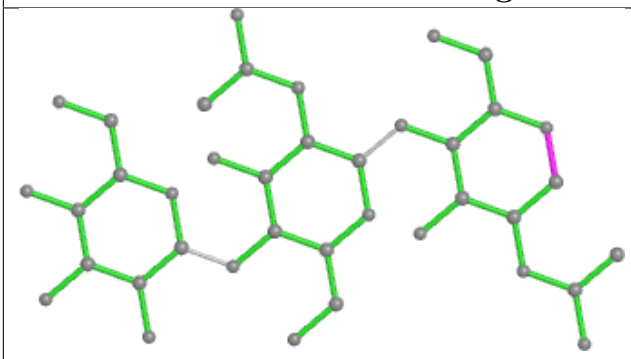


Torsions

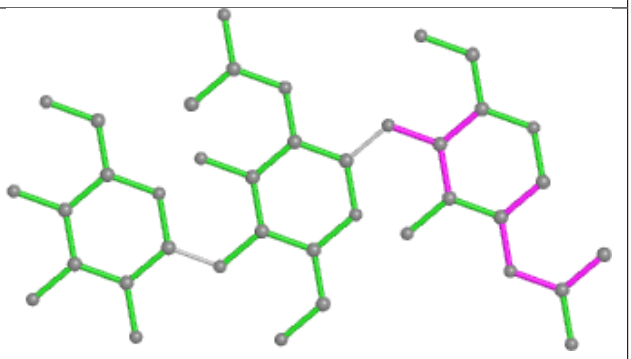


Rings

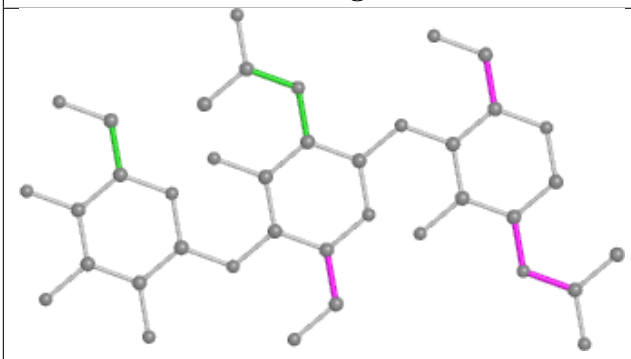
Oligosaccharide Chain T



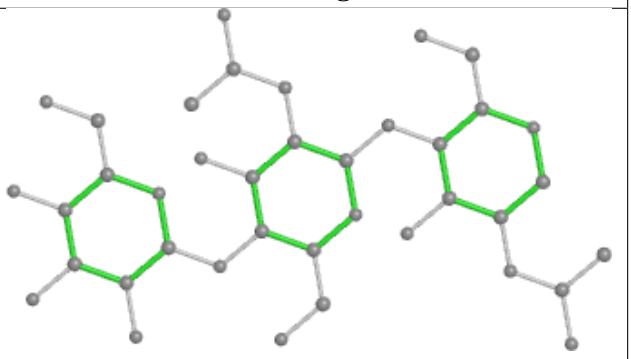
Bond lengths



Bond angles

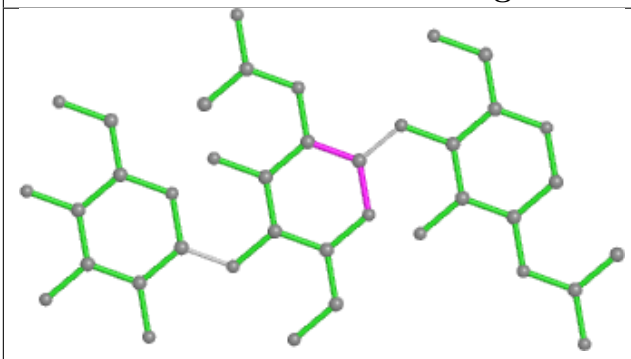


Torsions

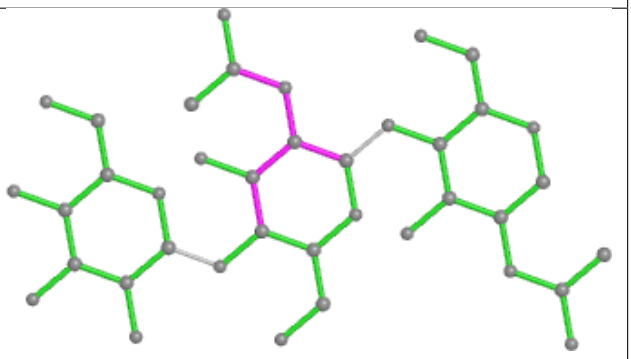


Rings

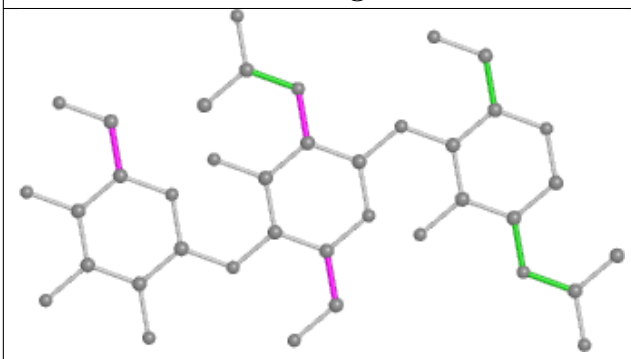
Oligosaccharide Chain V



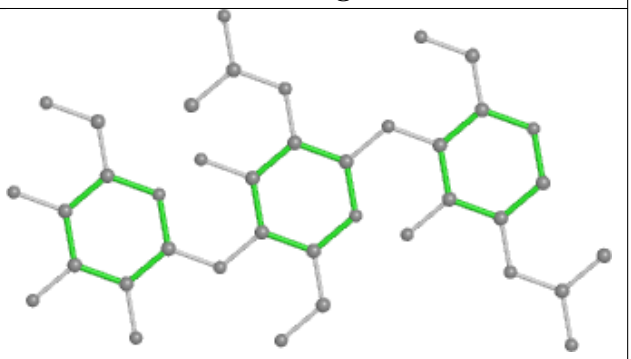
Bond lengths



Bond angles

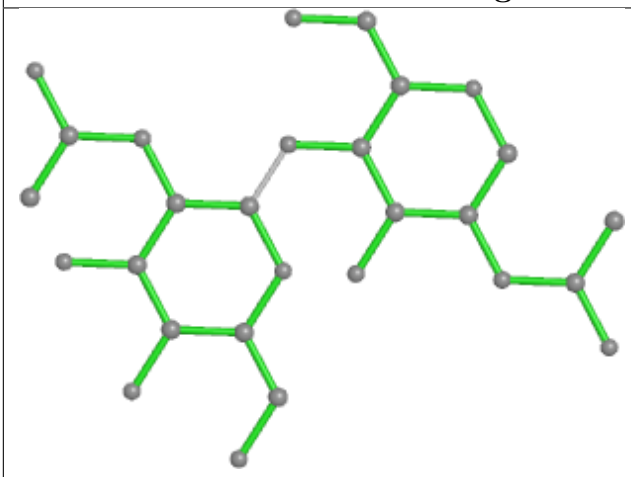


Torsions

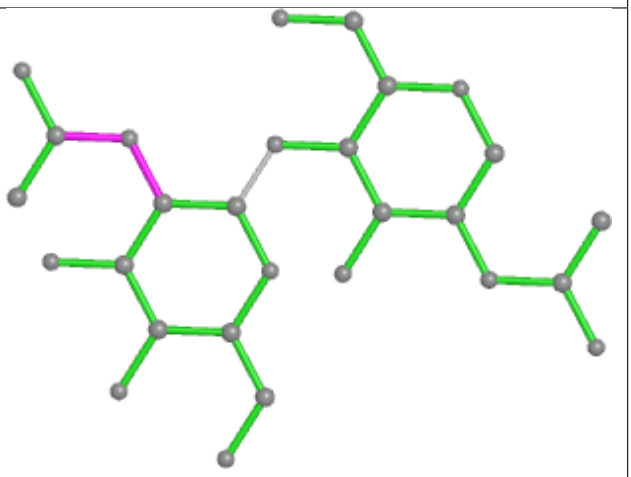


Rings

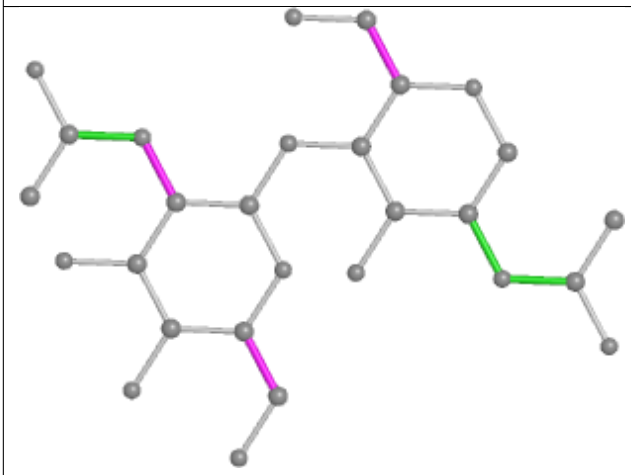
Oligosaccharide Chain R



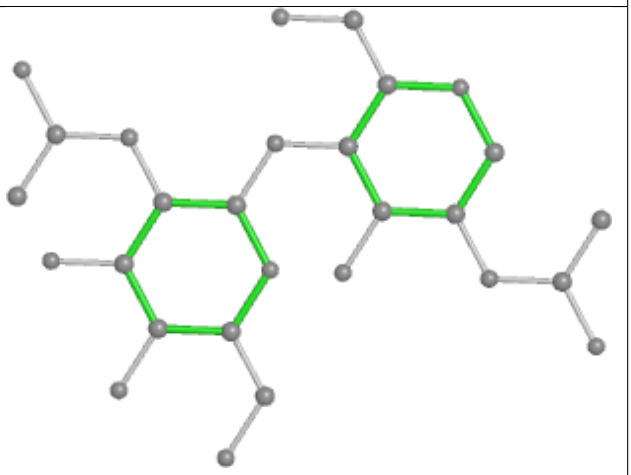
Bond lengths



Bond angles

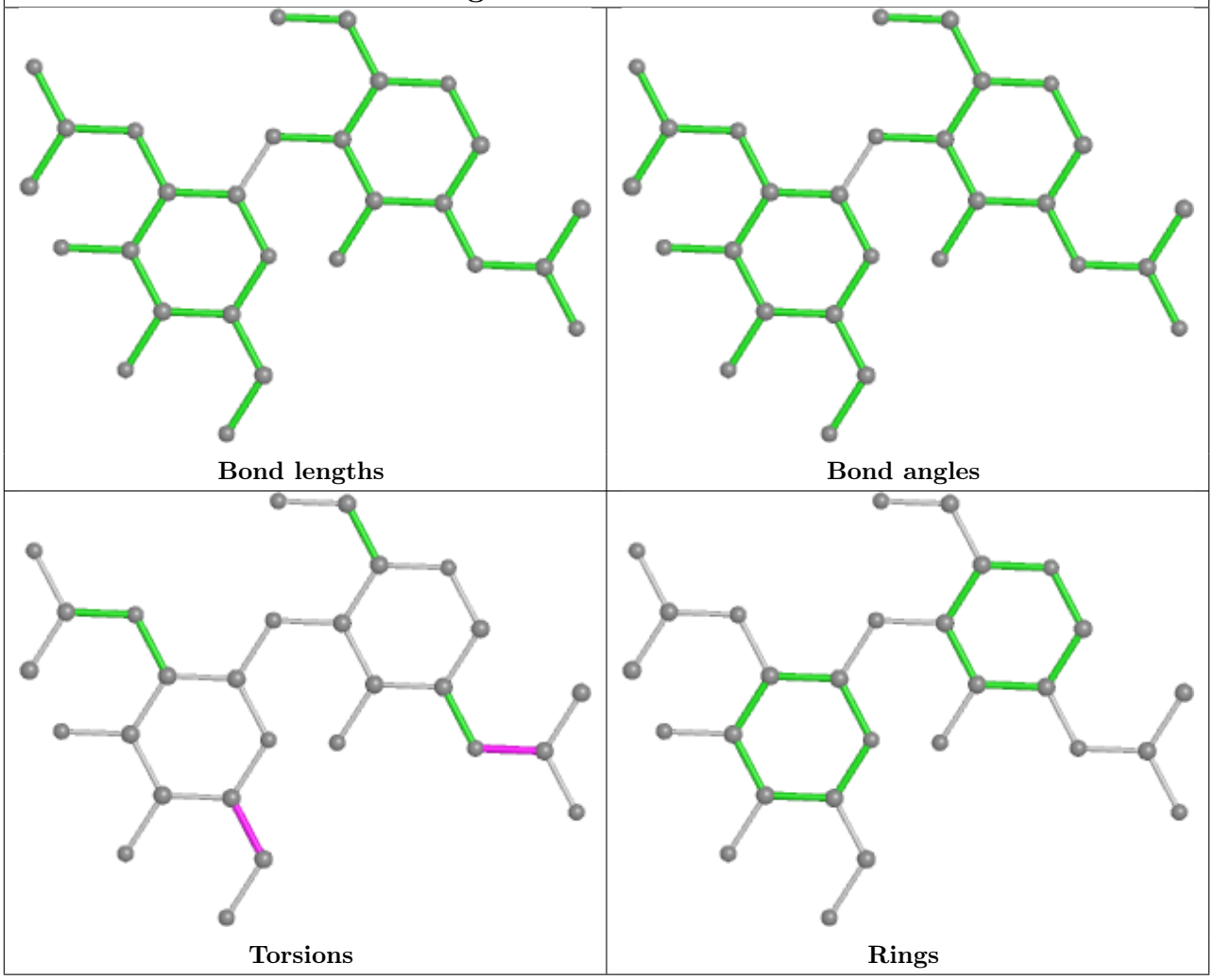


Torsions



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

All (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
11	A	901	ZK1	OAB-CAU	8.30	1.40	1.23
11	D	901	ZK1	OAB-CAU	8.26	1.40	1.23
11	C	901	ZK1	OAB-CAU	8.21	1.40	1.23
11	A	901	ZK1	CAW-NAY	-3.28	1.35	1.41
11	B	901	ZK1	CAW-NAY	-3.25	1.35	1.41
11	D	901	ZK1	CAW-NAY	-3.22	1.35	1.41
11	C	901	ZK1	CAW-NAY	-3.21	1.35	1.41
11	D	901	ZK1	CAV-NAP	-3.06	1.34	1.39
11	C	901	ZK1	CAV-NAP	-2.97	1.34	1.39
11	A	901	ZK1	CAV-NAP	-2.96	1.34	1.39
11	B	901	ZK1	CAV-NAP	-2.93	1.34	1.39
11	B	901	ZK1	CAU-NAY	-2.77	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	901	ZK1	CAU-NAY	-2.72	1.33	1.38
11	A	901	ZK1	CAU-NAY	-2.69	1.33	1.38
11	C	901	ZK1	CAU-NAY	-2.65	1.33	1.38
11	B	901	ZK1	CAV-CAW	-2.57	1.37	1.40
11	C	901	ZK1	CAV-CAW	-2.53	1.37	1.40
11	A	901	ZK1	CAV-CAW	-2.52	1.37	1.40
11	D	901	ZK1	CAV-CAW	-2.40	1.37	1.40
11	D	901	ZK1	CAT-NAP	-2.21	1.32	1.35
11	C	901	ZK1	CAT-NAP	-2.21	1.32	1.35
11	B	901	ZK1	CAT-NAP	-2.20	1.32	1.35
11	C	901	ZK1	CAR-NAX	2.19	1.46	1.41
11	A	901	ZK1	CAR-NAX	2.16	1.46	1.41
11	B	901	ZK1	CAR-NAX	2.14	1.46	1.41
11	A	901	ZK1	PBA-CAO	2.11	1.86	1.81
11	D	901	ZK1	CAR-NAX	2.11	1.45	1.41
11	B	901	ZK1	PBA-CAO	2.10	1.86	1.81
11	A	901	ZK1	CAT-NAP	-2.08	1.33	1.35
11	D	901	ZK1	PBA-CAO	2.08	1.86	1.81
11	C	901	ZK1	PBA-CAO	2.08	1.86	1.81

All (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
11	B	901	ZK1	CAI-CAR-NAX	-3.81	116.89	122.52
11	D	901	ZK1	CAI-CAR-NAX	-3.80	116.90	122.52
11	D	901	ZK1	CAV-NAP-CAT	-3.79	119.98	124.80
11	B	901	ZK1	CAV-NAP-CAT	-3.77	120.00	124.80
11	C	901	ZK1	CAV-NAP-CAT	-3.75	120.03	124.80
11	A	901	ZK1	CAI-CAR-NAX	-3.53	117.29	122.52
11	C	901	ZK1	CAI-CAR-NAX	-3.49	117.35	122.52
11	D	901	ZK1	CAO-NAY-CAU	3.28	119.71	116.51
11	B	901	ZK1	CAO-NAY-CAU	3.26	119.69	116.51
11	B	901	ZK1	CAS-CAR-NAX	3.11	123.48	119.92
11	D	901	ZK1	CAS-CAR-NAX	3.05	123.42	119.92
11	C	901	ZK1	CAO-NAY-CAU	3.03	119.47	116.51
11	A	901	ZK1	CAO-NAY-CAU	2.96	119.39	116.51
11	A	901	ZK1	CAS-CAR-NAX	2.93	123.28	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	901	ZK1	CAS-CAR-NAX	2.86	123.19	119.92
11	D	901	ZK1	CAU-CAT-NAP	2.71	120.29	117.49
11	D	901	ZK1	CAW-NAY-CAU	-2.62	119.54	122.79
11	A	901	ZK1	FAG-CAZ-CAS	-2.62	108.14	112.70
11	C	901	ZK1	CAU-CAT-NAP	2.62	120.19	117.49
11	B	901	ZK1	CAW-NAY-CAU	-2.62	119.55	122.79
11	B	901	ZK1	CAU-CAT-NAP	2.61	120.17	117.49
11	C	901	ZK1	FAG-CAZ-CAS	-2.59	108.19	112.70
11	A	901	ZK1	CAU-CAT-NAP	2.57	120.14	117.49
11	C	901	ZK1	CAW-NAY-CAU	-2.53	119.66	122.79
11	A	901	ZK1	CAW-NAY-CAU	-2.49	119.71	122.79
11	A	901	ZK1	CAT-CAU-NAY	2.46	120.14	117.32
11	B	901	ZK1	CAT-CAU-NAY	2.46	120.14	117.32
11	D	901	ZK1	FAG-CAZ-CAS	-2.42	108.49	112.70
11	B	901	ZK1	FAG-CAZ-CAS	-2.41	108.50	112.70
11	D	901	ZK1	CAT-CAU-NAY	2.40	120.07	117.32
11	C	901	ZK1	CAT-CAU-NAY	2.38	120.05	117.32

There are no chirality outliers.

All (19) torsion outliers are listed below:

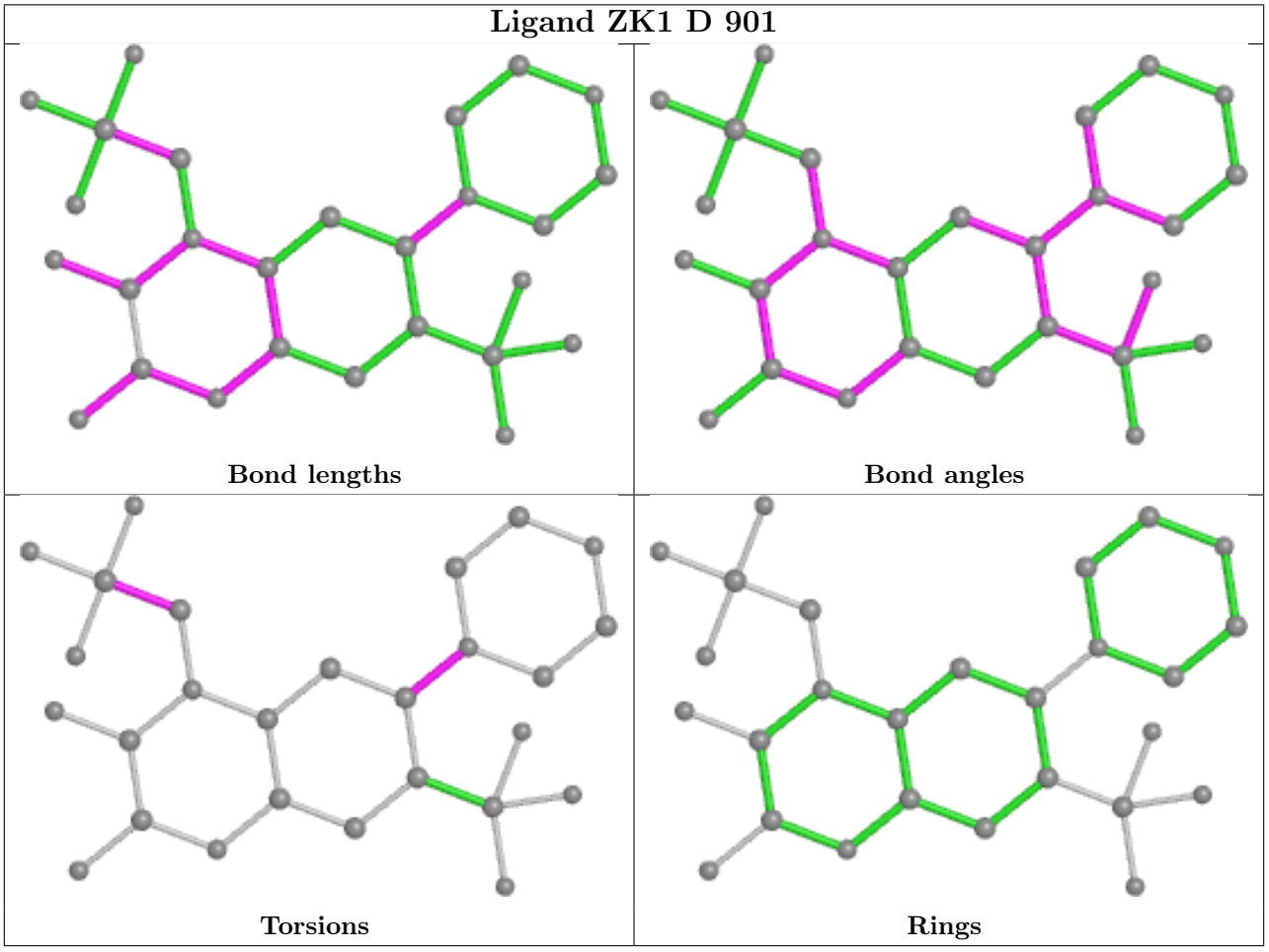
Mol	Chain	Res	Type	Atoms
11	B	901	ZK1	NAY-CAO-PBA-OAD
11	B	901	ZK1	NAY-CAO-PBA-OAE
11	D	901	ZK1	NAY-CAO-PBA-OAD
11	D	901	ZK1	NAY-CAO-PBA-OAE
12	A	905	NAG	C4-C5-C6-O6
12	A	905	NAG	O5-C5-C6-O6
11	B	901	ZK1	NAY-CAO-PBA-OAC
11	D	901	ZK1	NAY-CAO-PBA-OAC
11	A	901	ZK1	CAI-CAR-NAX-CAN
11	C	901	ZK1	CAI-CAR-NAX-CAN
11	B	901	ZK1	CAI-CAR-NAX-CAM
11	D	901	ZK1	CAI-CAR-NAX-CAM
11	D	901	ZK1	CAI-CAR-NAX-CAN
11	B	901	ZK1	CAI-CAR-NAX-CAN
11	A	901	ZK1	NAY-CAO-PBA-OAD
11	A	901	ZK1	NAY-CAO-PBA-OAE
11	C	901	ZK1	NAY-CAO-PBA-OAD
11	C	901	ZK1	NAY-CAO-PBA-OAE
12	B	905	NAG	C4-C5-C6-O6

There are no ring outliers.

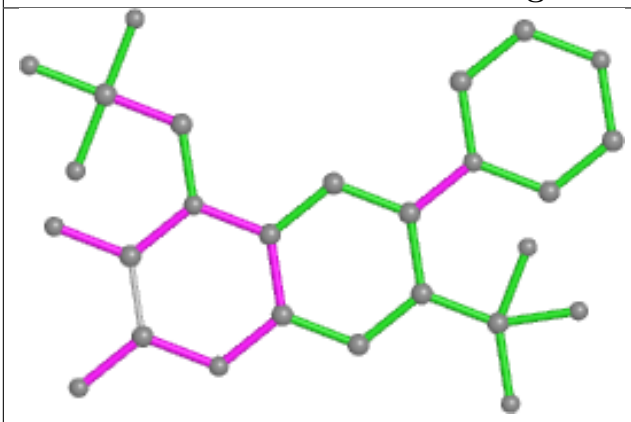
3 monomers are involved in 3 short contacts:

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

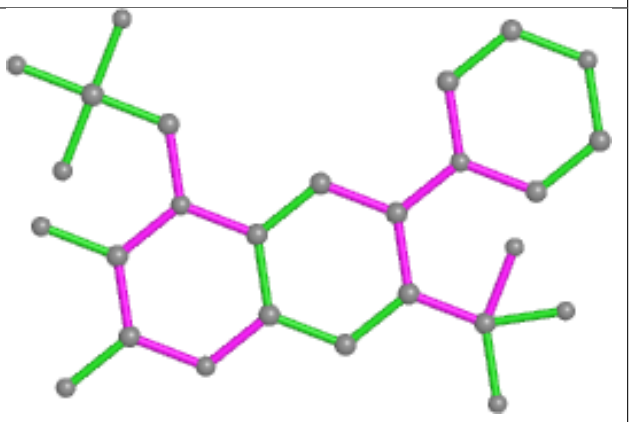
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



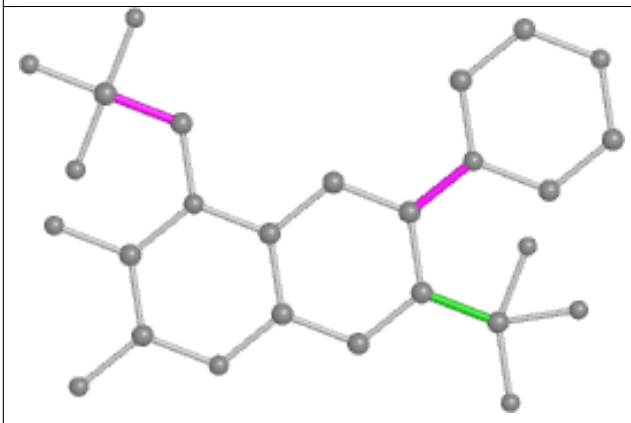
Ligand ZK1 A 901



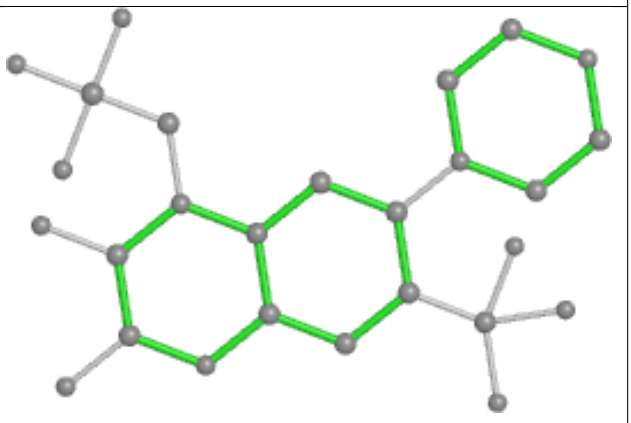
Bond lengths



Bond angles

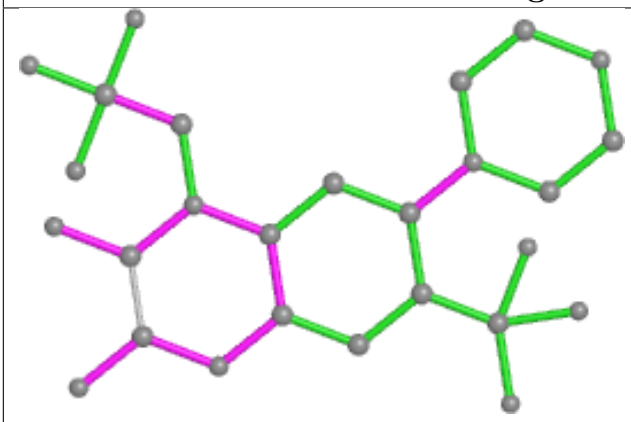


Torsions

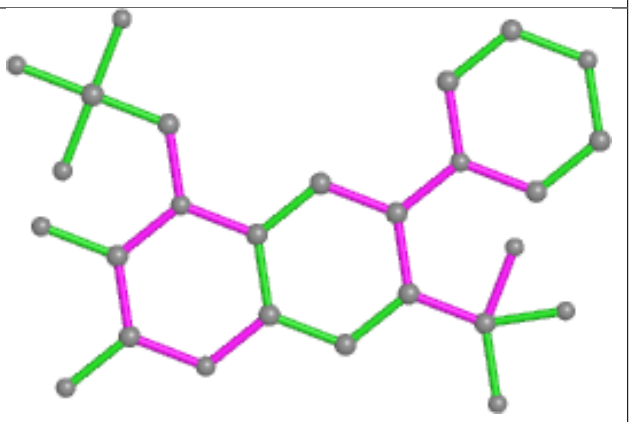


Rings

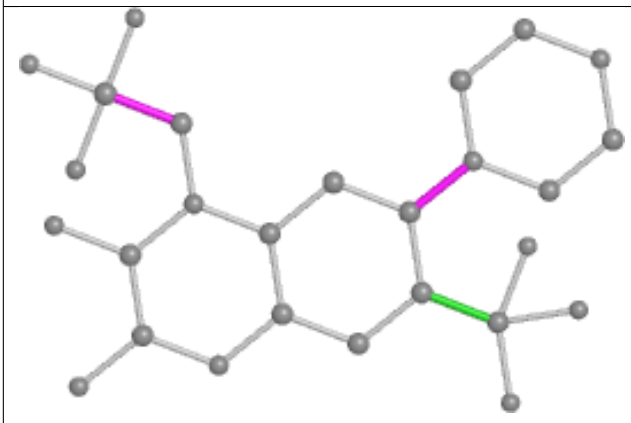
Ligand ZK1 B 901



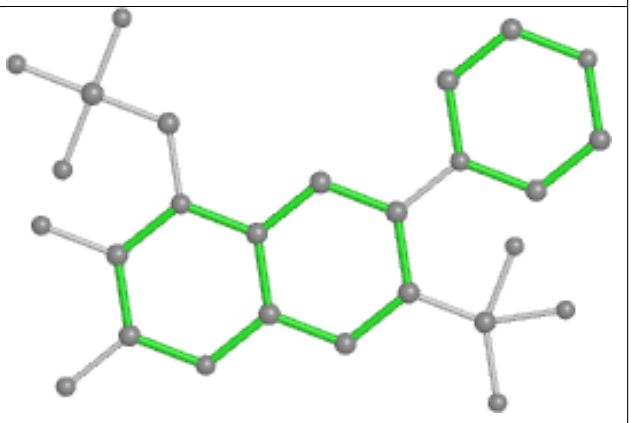
Bond lengths



Bond angles

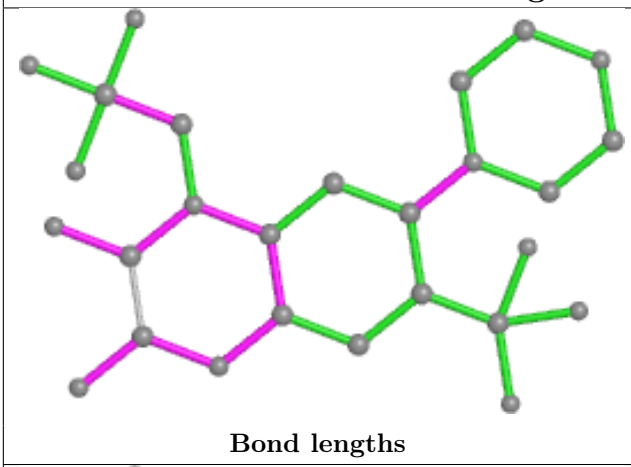


Torsions

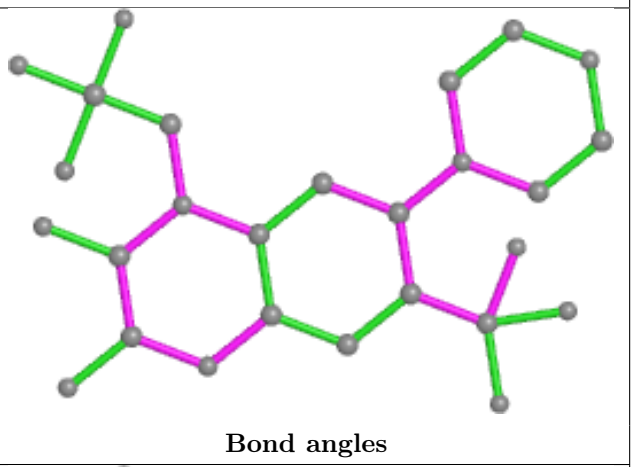


Rings

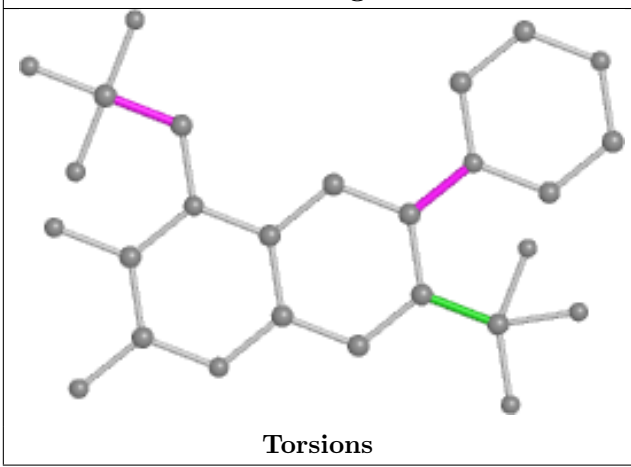
Ligand ZK1 C 901



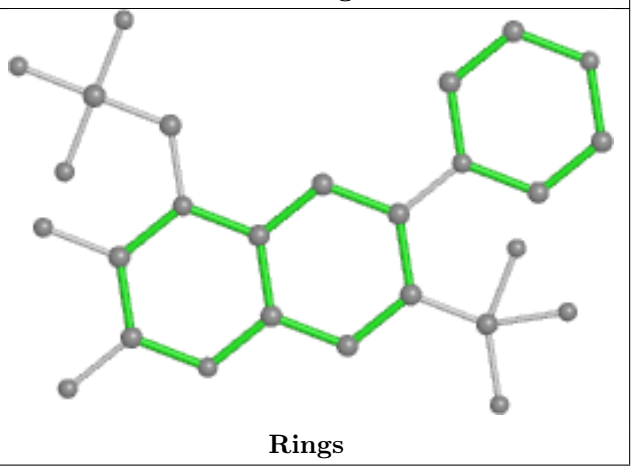
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	3
3	E	3

All 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
1	E	88:UNK	C	89:UNK	N	13.45

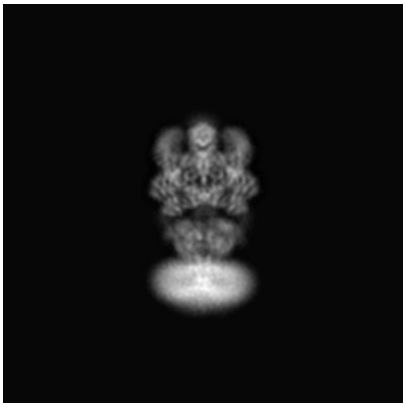
6 Map visualisation

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.

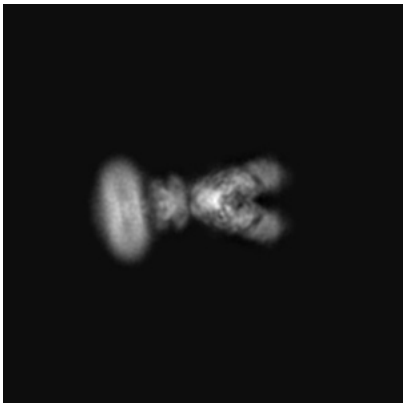
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

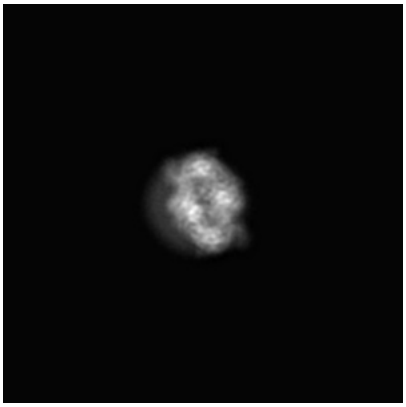
6.1.1 Primary map



X



Y



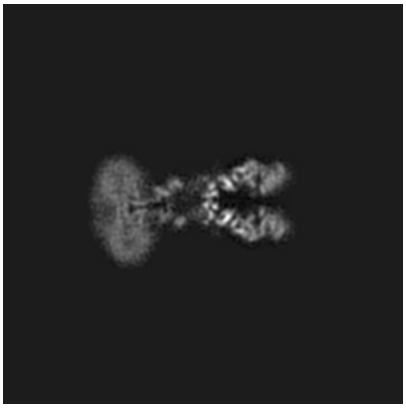
Z

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

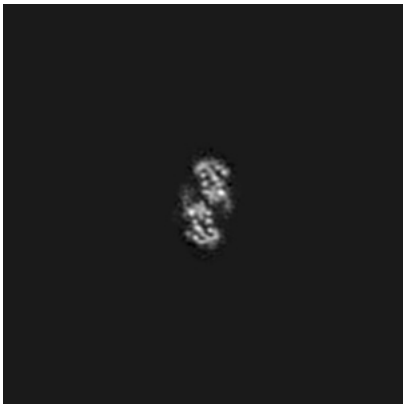
6.2 Central slices

6.2.1 Primary map

X Index: 160



Y Index: 160



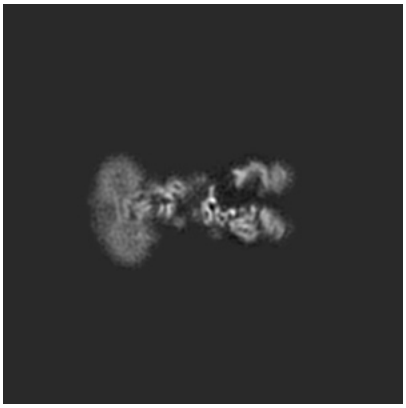
Z Index: 160

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

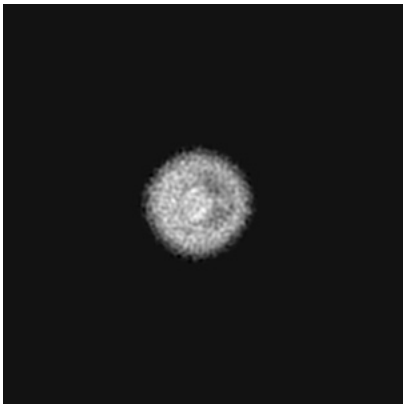
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 157



Y Index: 157

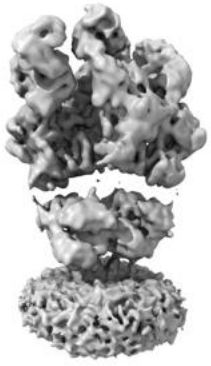


Z Index: 91

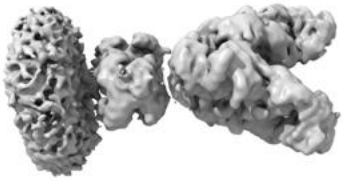
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

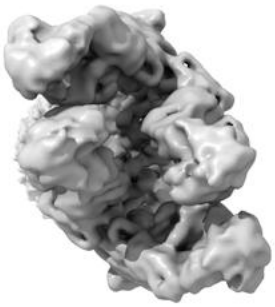
6.4.1 Primary map



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.

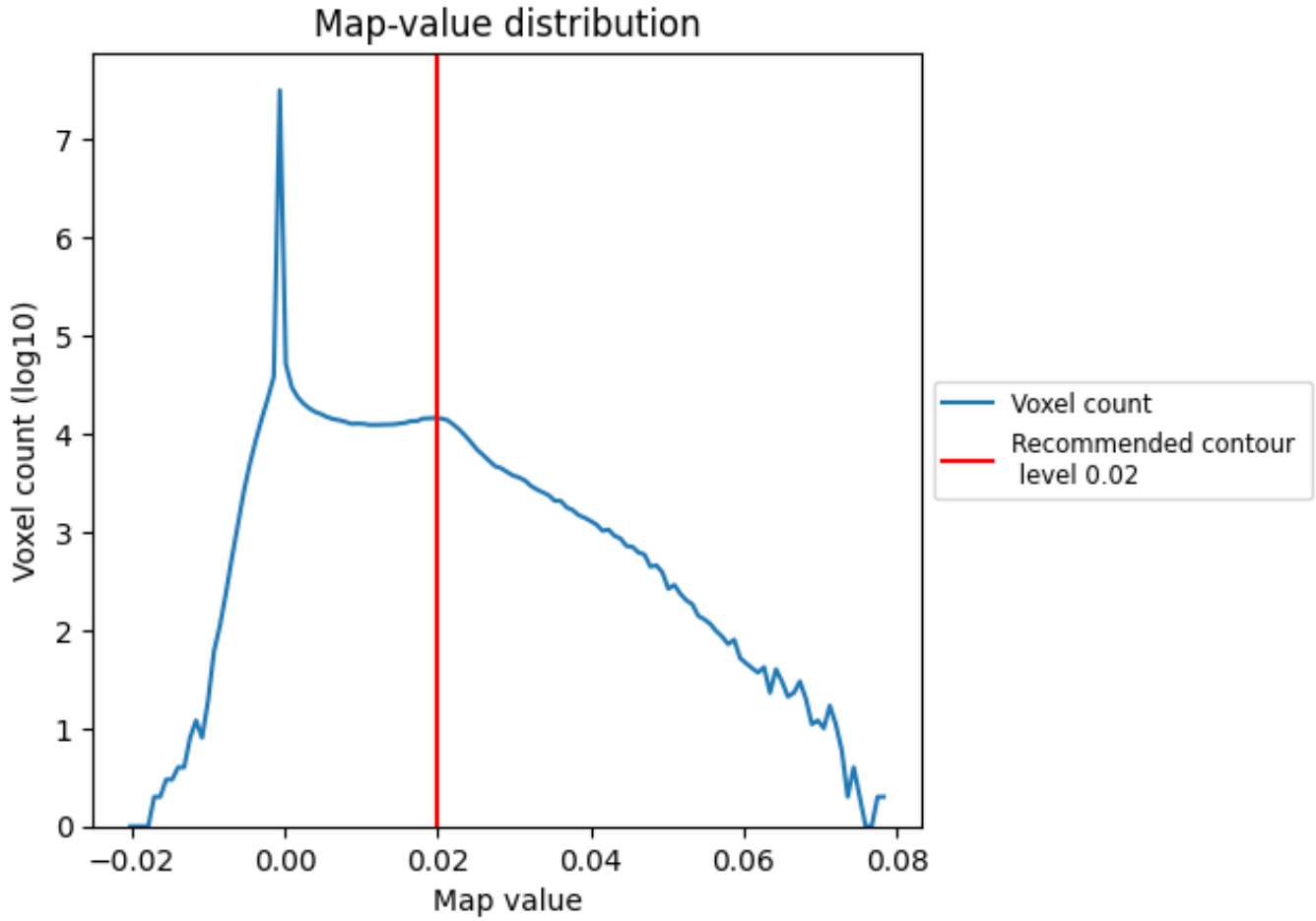
6.5 Mask visualisation (i)

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

7 Map analysis

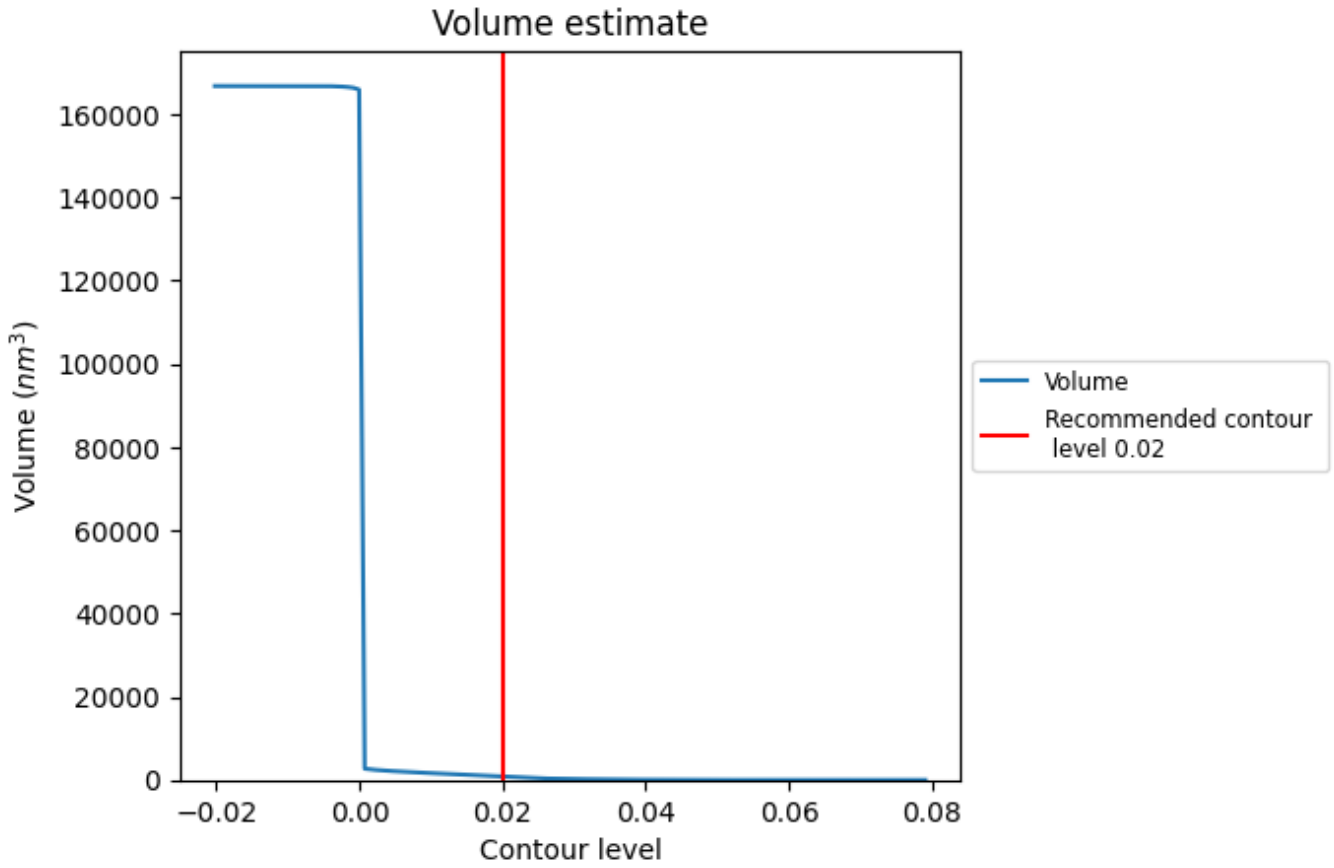
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

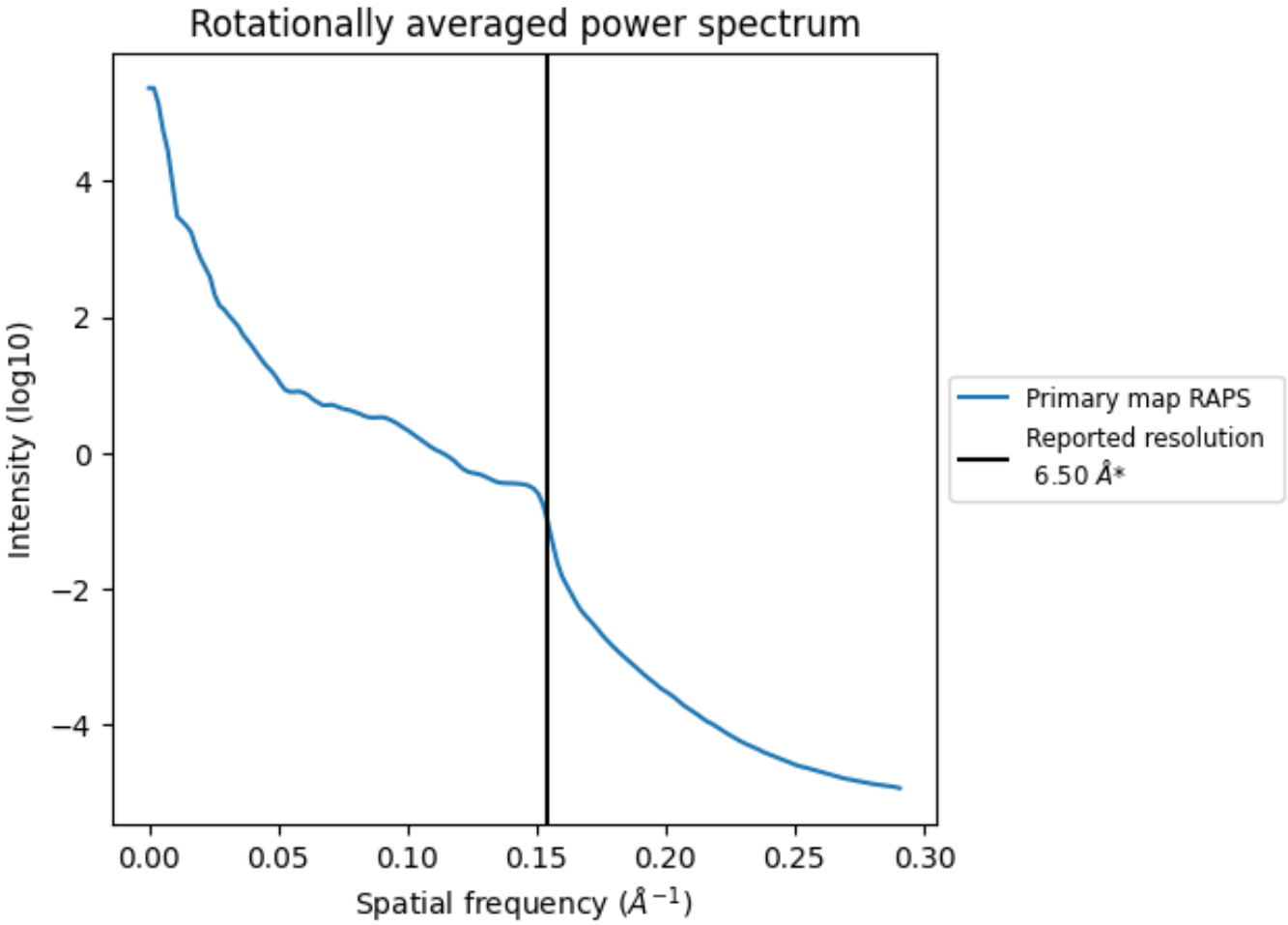
7.2 Volume estimate



The volume at the recommended contour level is 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}

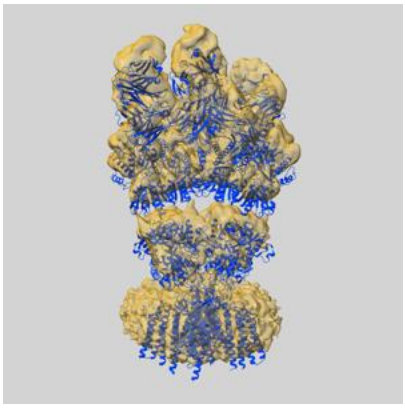
8 Fourier-Shell correlation

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

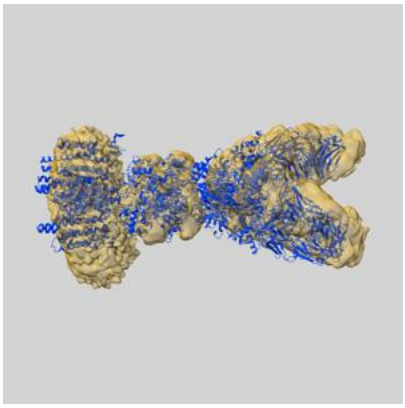
9 Map-model fit

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.

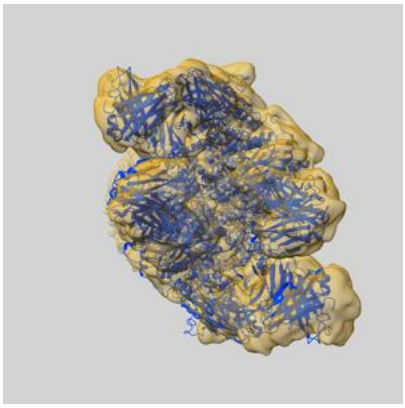
9.1 Map-model overlay



X



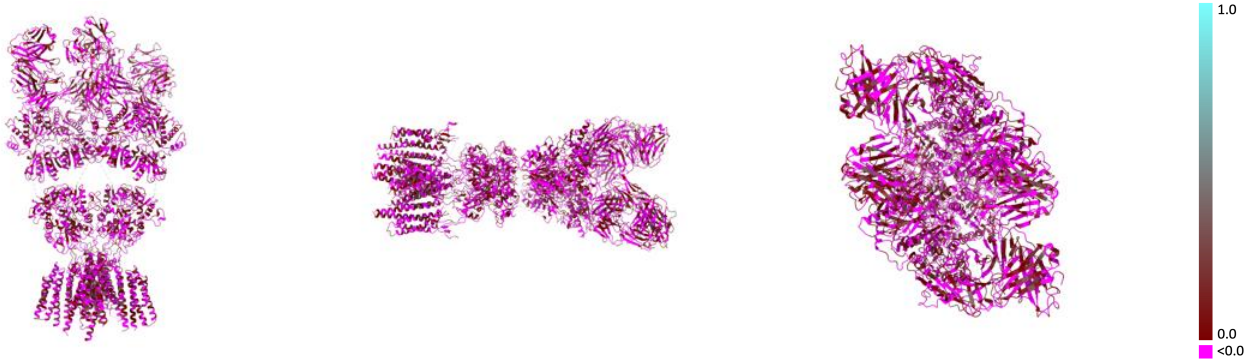
Y



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.

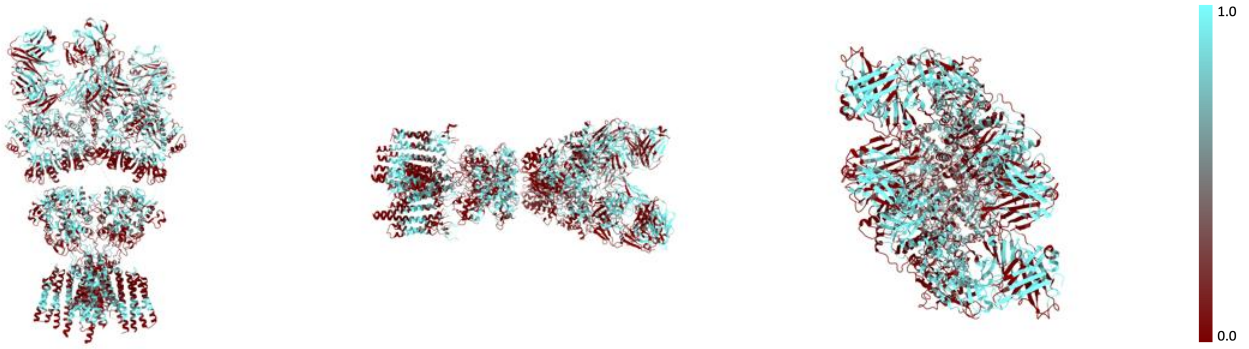
9.2 Q-score mapped to coordinate model (i)



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.

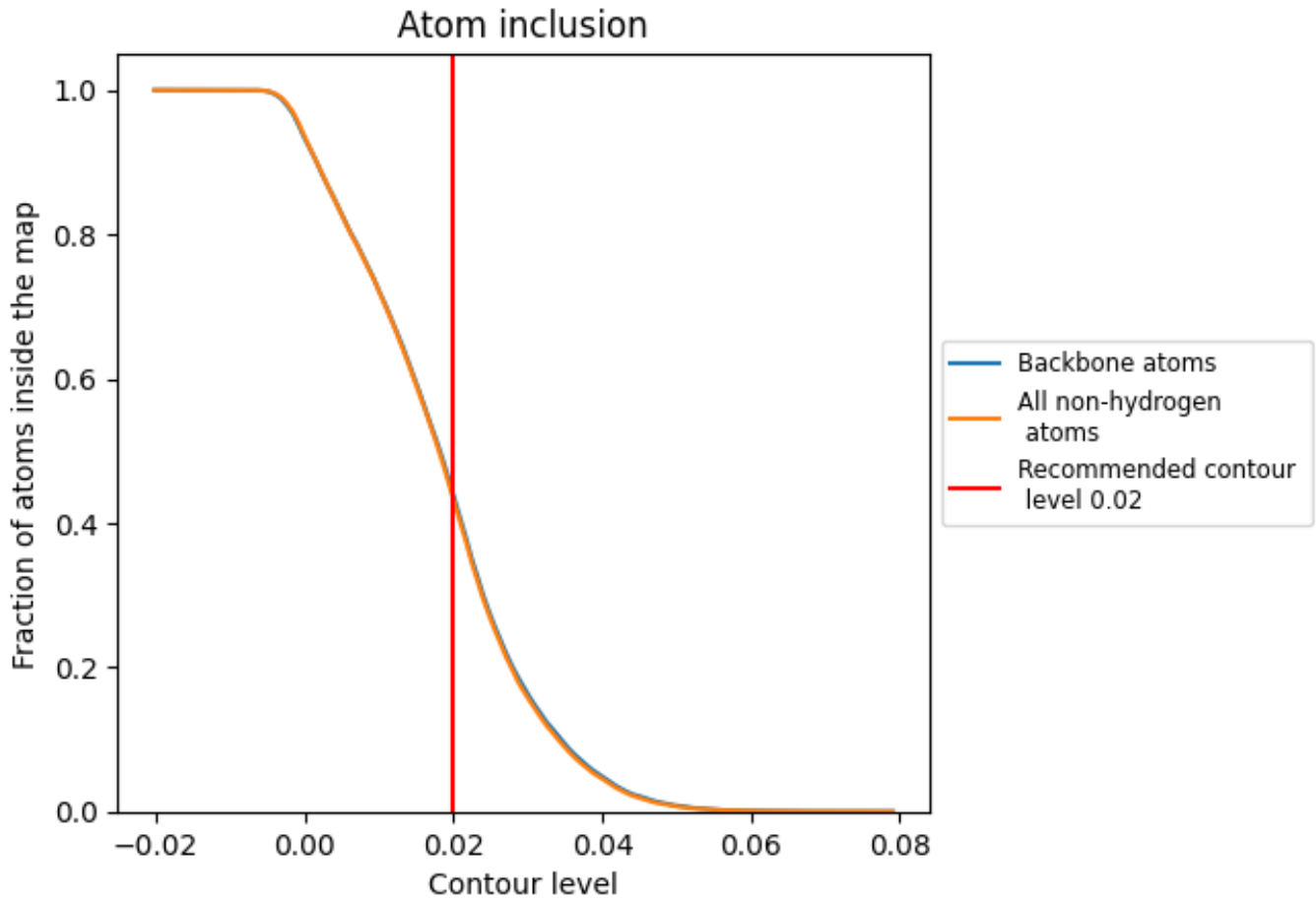
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

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

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