



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 11:46 PM EST

PDB ID : 6NJJ
EMDB ID : EMD-9389
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

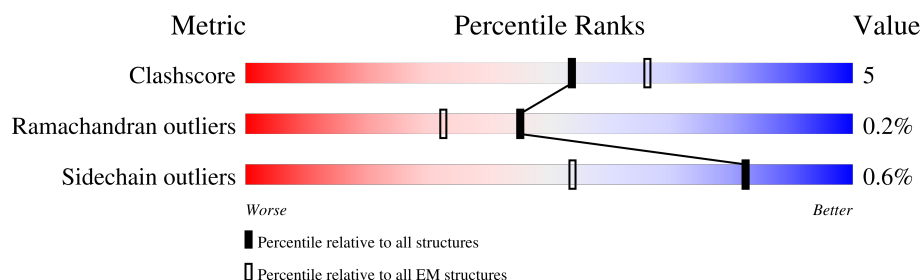
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	907	<div> <div>43%</div> <div>74%</div> <div>12%</div> <div>13%</div> </div>
2	B	883	<div> <div>41%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
2	D	883	<div> <div>41%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>
3	C	888	<div> <div>38%</div> <div>78%</div> <div>10%</div> <div>12%</div> </div>
4	E	153	<div> <div>48%</div> <div>76%</div> <div>24%</div> </div>
4	G	153	<div> <div>48%</div> <div>76%</div> <div>24%</div> </div>
5	F	323	<div> <div>38%</div> <div>50%</div> <div>48%</div> </div>
5	H	323	<div> <div>37%</div> <div>50%</div> <div>48%</div> </div>

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Mol	Chain	Length	Quality of chain
6	I	257	
7	J	225	
7	N	225	
8	K	262	
8	O	262	
9	L	224	
9	M	224	
10	P	3	
10	Q	3	
10	T	3	
10	U	3	
10	V	3	
11	R	2	
11	S	2	
11	W	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	R	1	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34410 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	785	Total	C	N	O	S	0	0
			5978	3843	990	1114	31		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	743	GLY	ARG	conflict	UNP P19490
A	744	ALA	GLY	conflict	UNP P19490
A	754	ALA	SER	conflict	UNP P19490
A	758	ALA	VAL	conflict	UNP P19490
A	764	ALA	SER	conflict	UNP P19490

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	782	Total	C	N	O	S	0	0
			5678	3661	905	1087	25		
2	D	782	Total	C	N	O	S	0	0
			5682	3664	906	1087	25		

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 Glutamate receptor 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	784	Total	C	N	O	S	0	0
			6002	3862	990	1116	34		

- Molecule 4 is a protein called A'-C' auxiliary proteins.

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

- Molecule 5 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

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

- Molecule 6 is a protein called 11B8 scFv.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	224	Total	C	N	O		0	0
			1100	652	224	224			

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

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

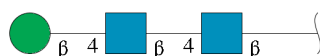
- Molecule 8 is a protein called 15F1 Fab heavy chain.

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

- Molecule 9 is a protein called 5B2 Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	218	Total	C	N	O	0	0
			1090	654	218	218		
9	M	213	Total	C	N	O	0	0
			1065	639	213	213		

- Molecule 10 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.



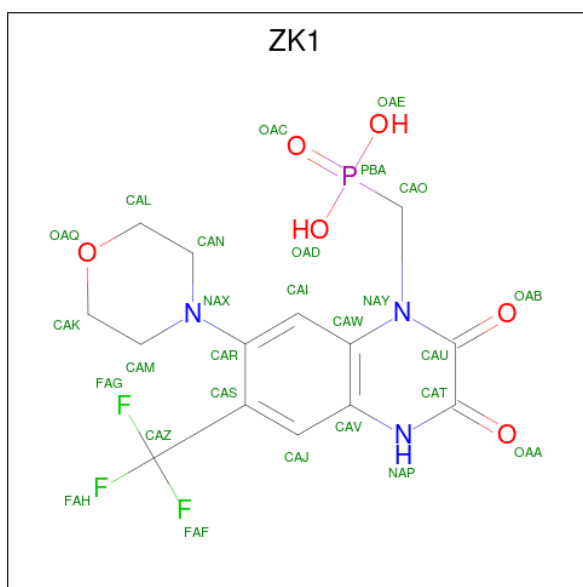
Mol	Chain	Residues	Atoms				AltConf	Trace
10	P	3	Total	C	N	O	0	0
			39	22	2	15		
10	Q	3	Total	C	N	O	0	0
			39	22	2	15		
10	T	3	Total	C	N	O	0	0
			39	22	2	15		
10	U	3	Total	C	N	O	0	0
			39	22	2	15		
10	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



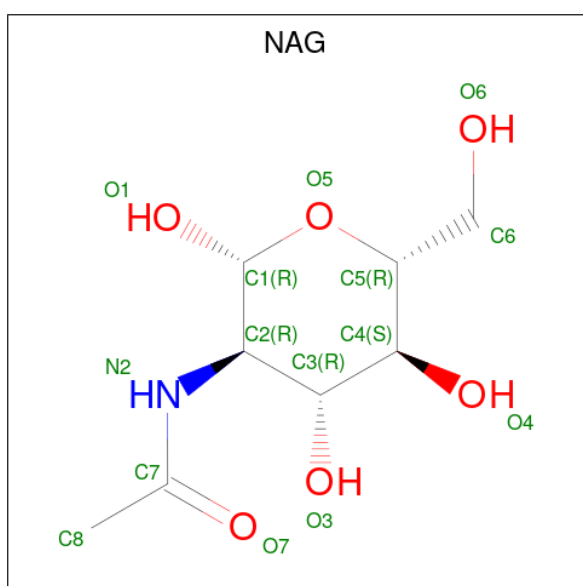
Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	2	Total	C	N	O	0	0
			28	16	2	10		
11	S	2	Total	C	N	O	0	0
			28	16	2	10		
11	W	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P).



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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

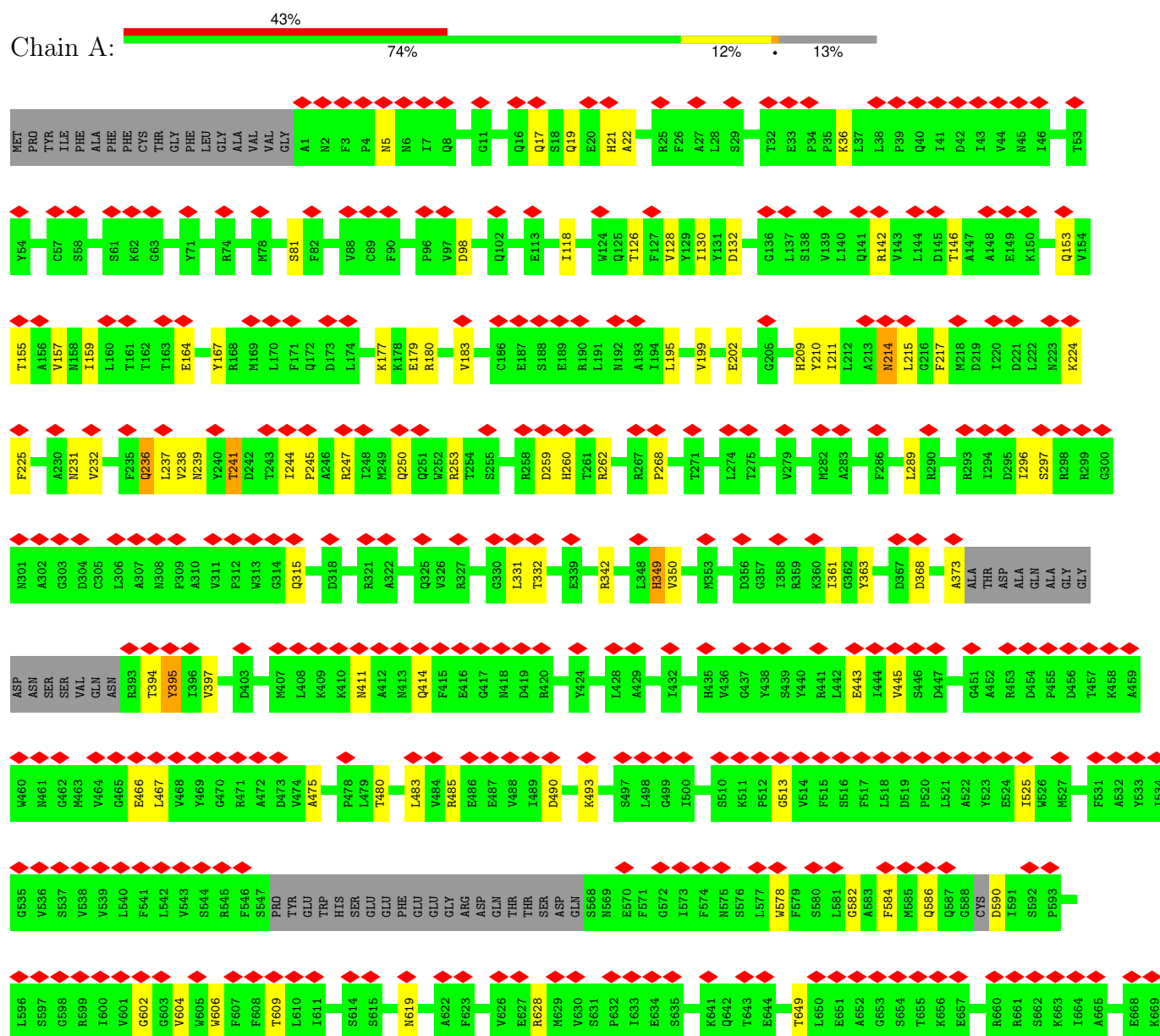


Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total 14	C 8	N 1	O 5	0
13	B	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0

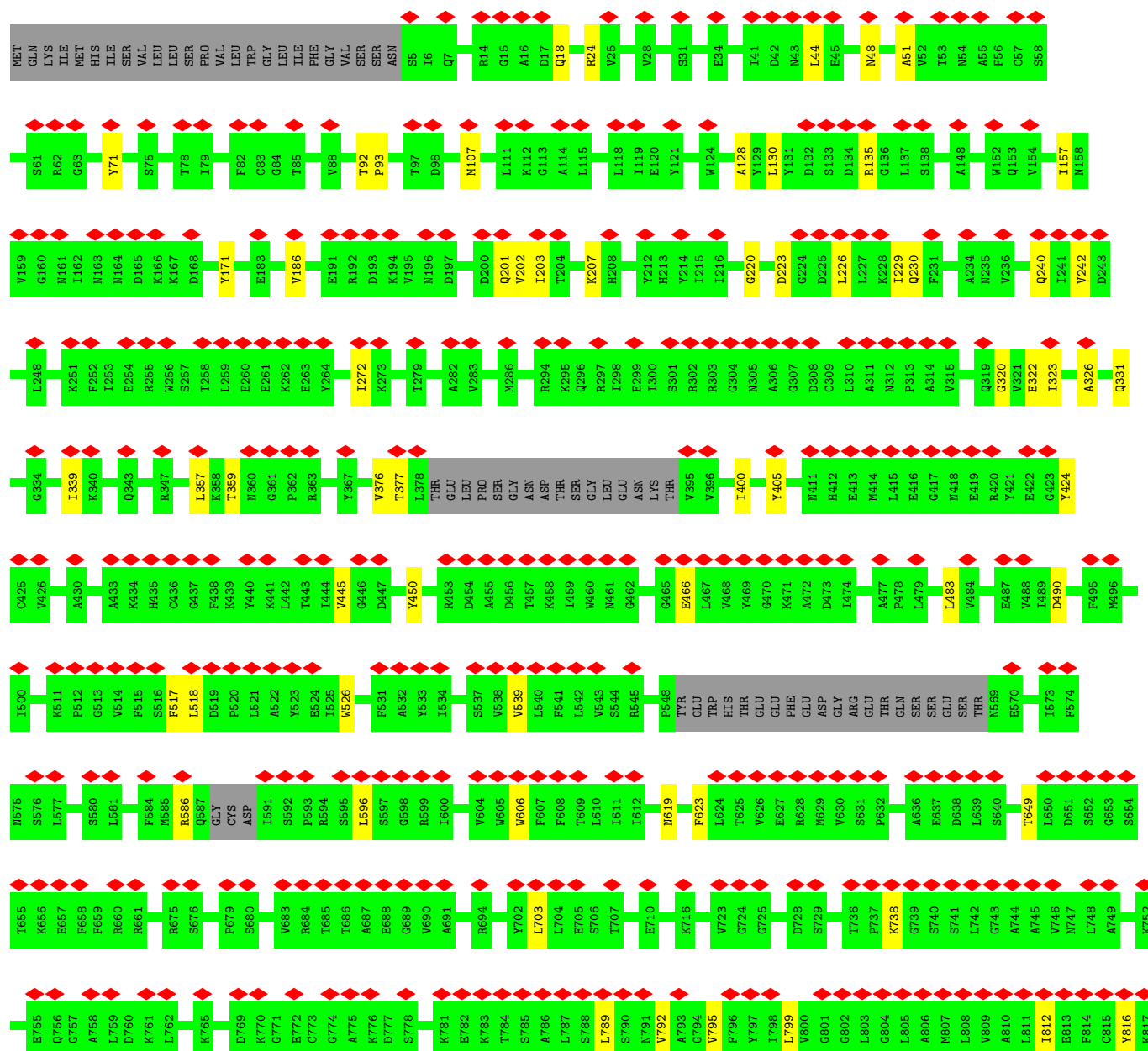
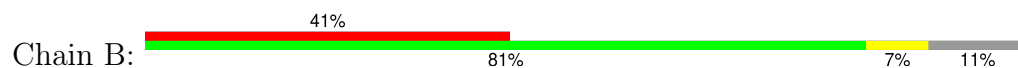
3 Residue-property plots

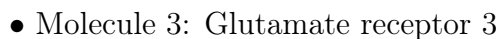
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

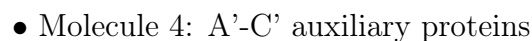
• Molecule 1: Glutamate receptor 1

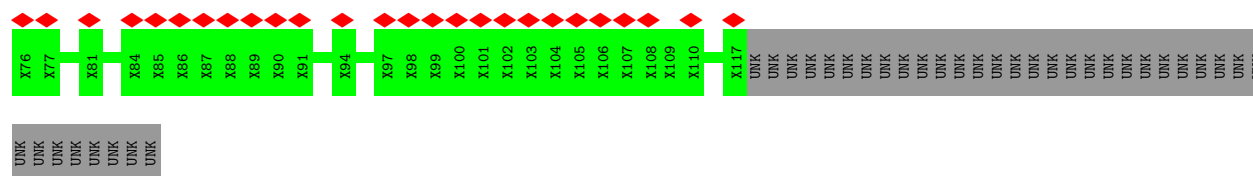


- Molecule 2: Glutamate receptor 2

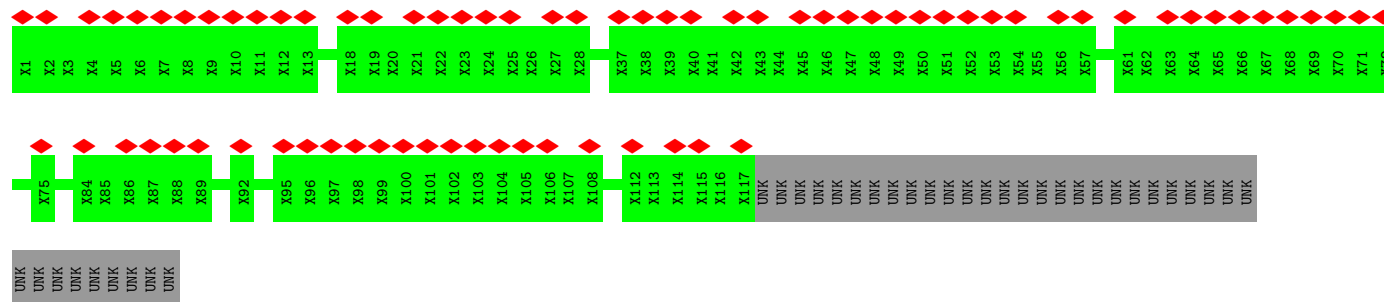




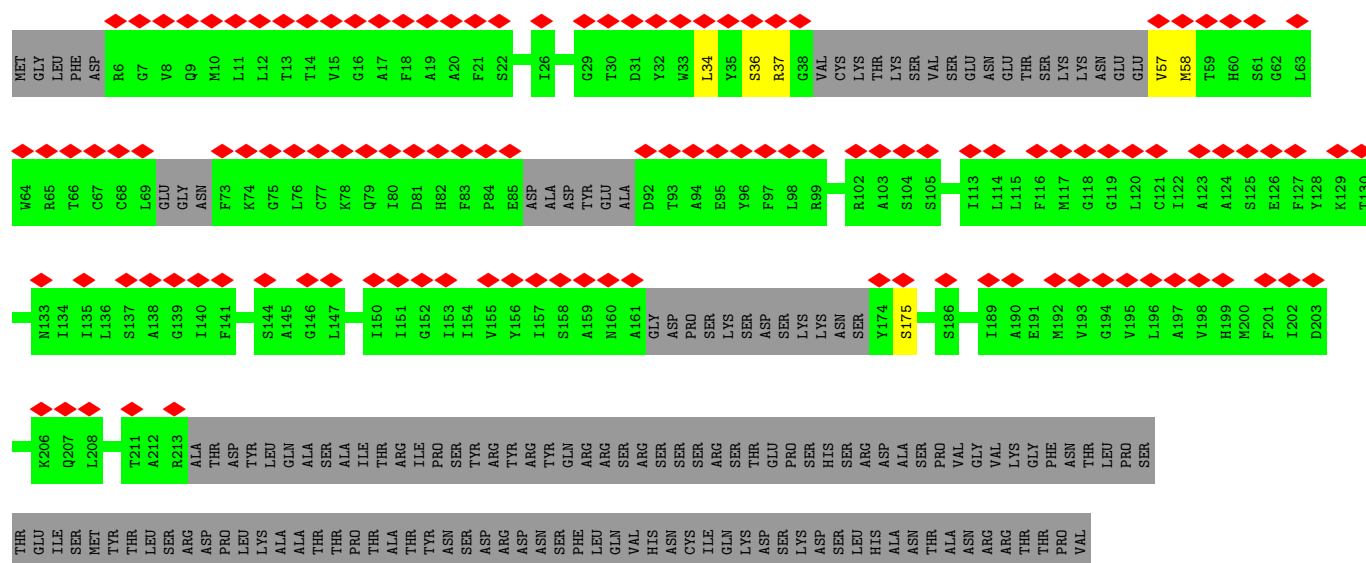
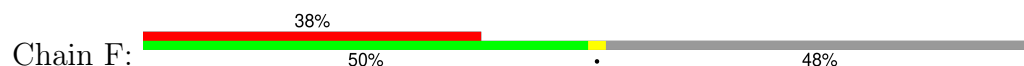




• Molecule 4: A'-C' auxiliary proteins

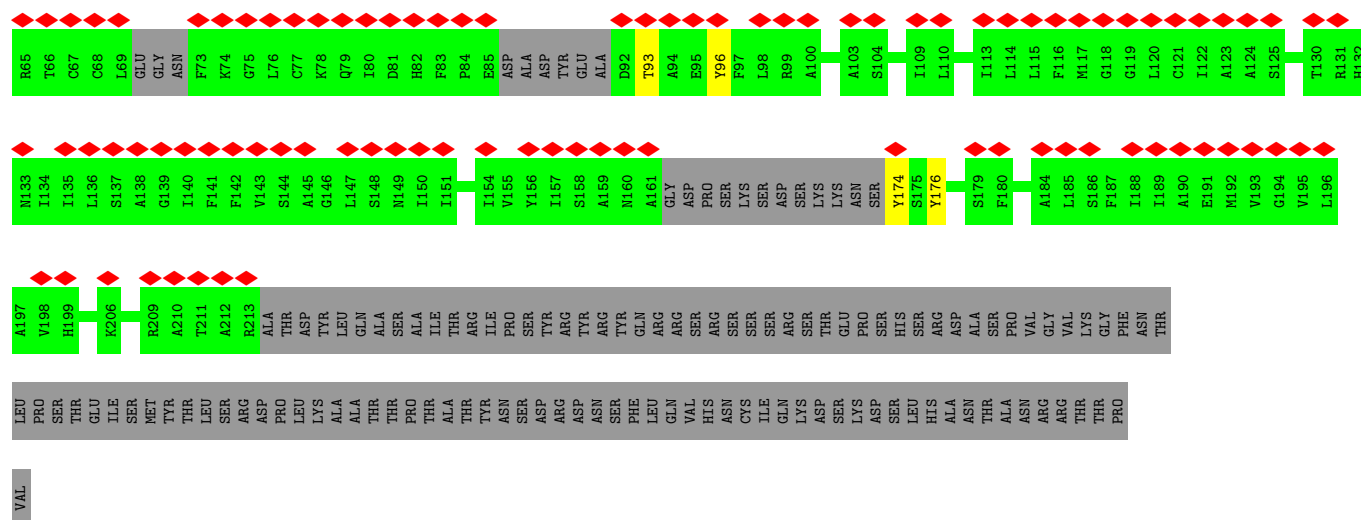


• Molecule 5: Voltage-dependent calcium channel gamma-2 subunit

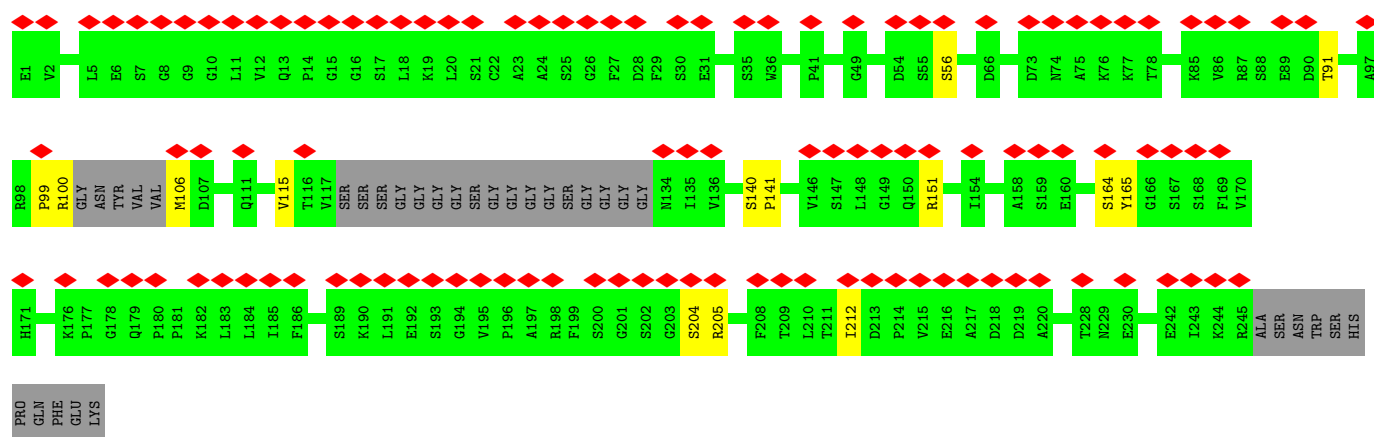
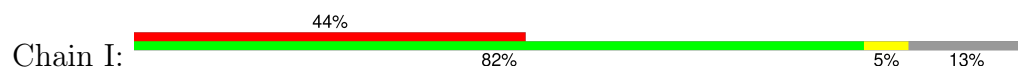


• Molecule 5: Voltage-dependent calcium channel gamma-2 subunit

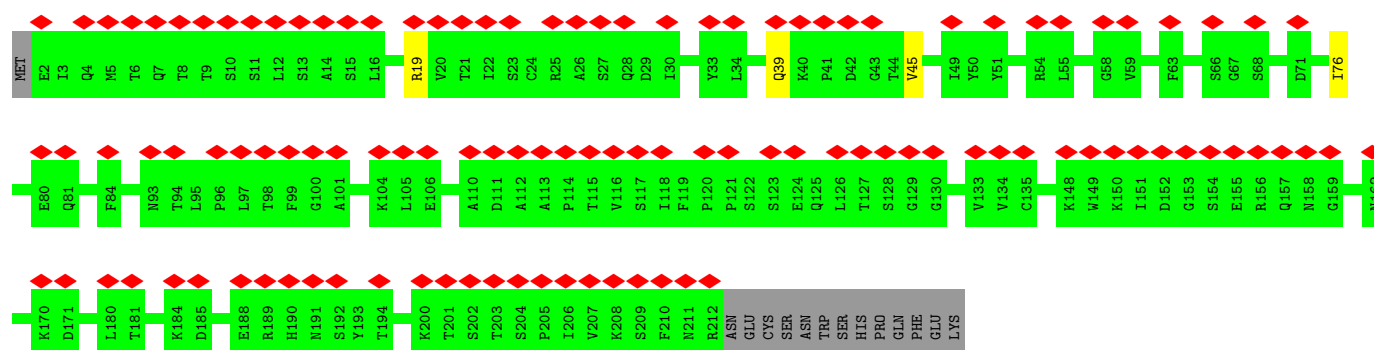
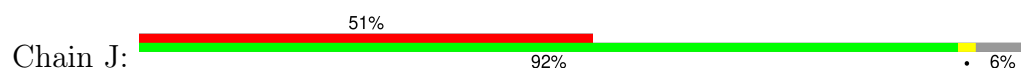




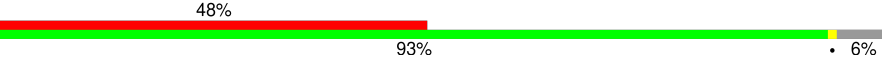
- Molecule 6: 11B8 scFv

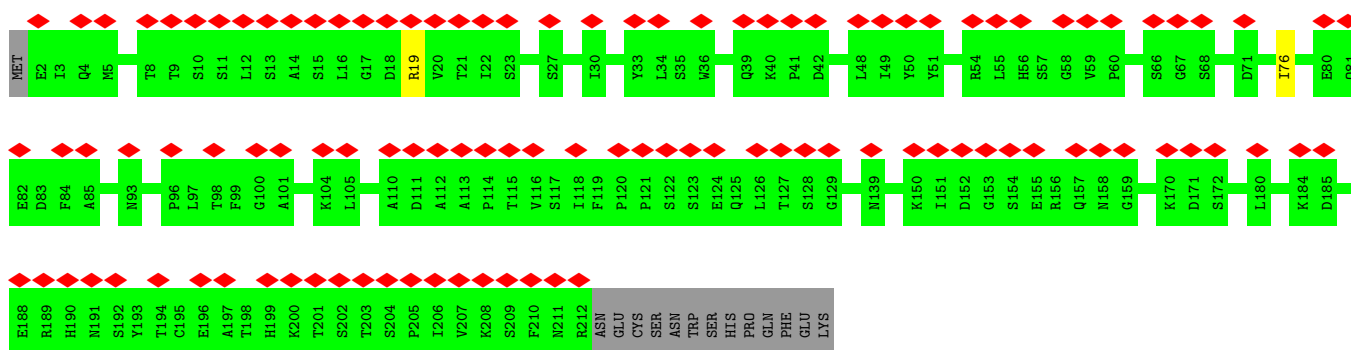


- Molecule 7: 15F1 Fab light chain




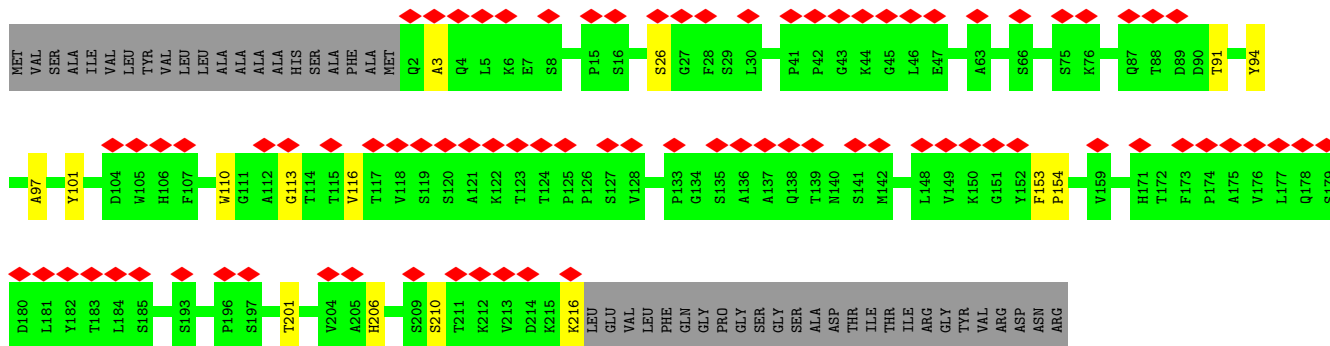
- Molecule 7: 15F1 Fab light chain

Chain N: 




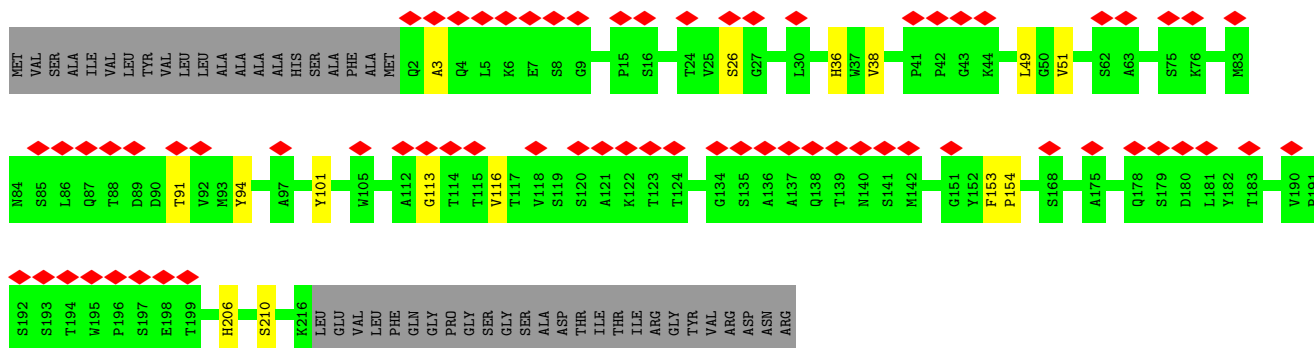
• Molecule 8: 15F1 Fab heavy chain

Chain K: 




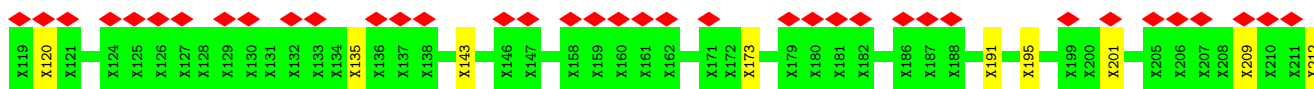
• Molecule 8: 15F1 Fab heavy chain

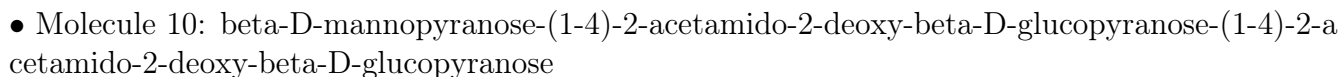
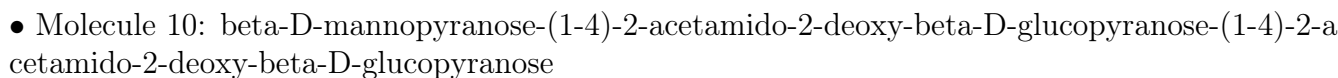
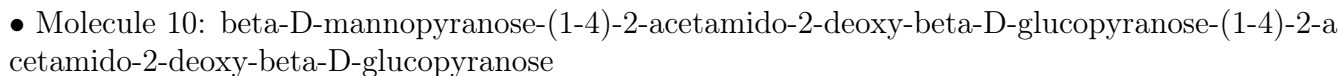
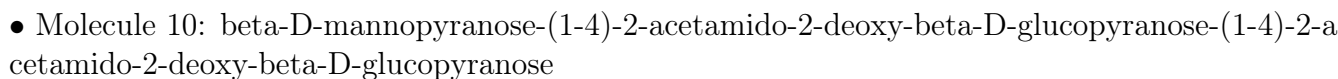
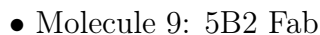
Chain O: 



• Molecule 9: 5B2 Fab

Chain L: 







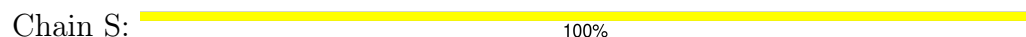
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161000	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 ($e^-/\text{\AA}^2$)	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	0.239	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.044	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, ZK1, BMA

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	0.27	0/6110	0.49	0/8310
2	B	0.27	0/5803	0.48	1/7941 (0.0%)
2	D	0.27	0/5807	0.48	1/7945 (0.0%)
3	C	0.28	0/6140	0.50	6/8350 (0.1%)
5	F	0.27	0/1021	0.42	0/1401
5	H	0.27	0/1021	0.42	0/1401
6	I	0.27	0/1097	0.48	0/1519
7	J	0.26	0/1041	0.48	0/1448
7	N	0.25	0/1041	0.48	0/1448
8	K	0.26	0/1058	0.50	0/1470
8	O	0.26	0/1058	0.50	0/1470
All	All	0.27	0/31197	0.48	8/42703 (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
1	A	0	1
6	I	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	455	PRO	CA-N-CD	-8.71	99.31	111.50
3	C	568	PRO	CA-N-CD	-8.51	99.58	111.50
2	B	596	LEU	CA-CB-CG	6.66	130.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	PRO	C-N-CA	6.62	138.26	121.70
2	D	596	LEU	CA-CB-CG	6.25	129.67	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	ASP	Peptide
6	I	204	SER	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	5978	0	5709	95	0
2	B	5678	0	5209	43	0
2	D	5682	0	5220	48	0
3	C	6002	0	5699	83	0
4	E	585	0	125	0	0
4	G	585	0	125	0	0
5	F	1007	0	718	3	0
5	H	1007	0	718	5	0
6	I	1100	0	501	16	0
7	J	1042	0	453	2	0
7	N	1042	0	453	1	0
8	K	1059	0	470	10	0
8	O	1059	0	470	8	0
9	L	1090	0	230	9	0
9	M	1065	0	224	9	0
10	P	39	0	34	0	0
10	Q	39	0	34	0	0
10	T	39	0	32	0	0
10	U	39	0	34	2	0
10	V	39	0	34	0	0
11	R	28	0	25	13	0
11	S	28	0	25	0	0
11	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	27	0	13	0	0
12	B	27	0	13	0	0
12	C	27	0	13	1	0
12	D	27	0	13	1	0
13	A	14	0	13	0	0
13	B	14	0	13	0	0
13	D	14	0	13	0	0
All	All	34410	0	26658	306	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 306 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)
11:R:1:NAG:C1	11:R:1:NAG:C2	1.79	1.57
1:A:241:THR:OG1	11:R:1:NAG:C1	1.65	1.42
1:A:394:THR:O	1:A:395:TYR:CD2	1.84	1.28
3:C:454:ASP:OD1	3:C:455:PRO:CD	1.82	1.27
3:C:568:PRO:CD	3:C:571:PHE:HB2	1.64	1.26

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	777/907 (86%)	724 (93%)	50 (6%)	3 (0%)	30	68
2	B	774/883 (88%)	743 (96%)	31 (4%)	0	100	100
2	D	774/883 (88%)	742 (96%)	32 (4%)	0	100	100
3	C	774/888 (87%)	734 (95%)	34 (4%)	6 (1%)	16	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	159/323 (49%)	153 (96%)	6 (4%)	0	100	100
5	H	159/323 (49%)	157 (99%)	2 (1%)	0	100	100
6	I	218/257 (85%)	208 (95%)	9 (4%)	1 (0%)	25	64
7	J	209/225 (93%)	207 (99%)	2 (1%)	0	100	100
7	N	209/225 (93%)	206 (99%)	3 (1%)	0	100	100
8	K	213/262 (81%)	208 (98%)	5 (2%)	0	100	100
8	O	213/262 (81%)	208 (98%)	5 (2%)	0	100	100
All	All	4479/5438 (82%)	4290 (96%)	179 (4%)	10 (0%)	45	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	780	SER
3	C	777	ASP
3	C	781	LYS
3	C	784	THR
1	A	777	ASP

5.3.2 Protein sidechains ⓘ

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	609/766 (80%)	602 (99%)	7 (1%)	70	80
2	B	551/753 (73%)	549 (100%)	2 (0%)	89	91
2	D	552/753 (73%)	550 (100%)	2 (0%)	89	91
3	C	616/766 (80%)	612 (99%)	4 (1%)	84	88
5	F	50/275 (18%)	50 (100%)	0	100	100
5	H	50/275 (18%)	50 (100%)	0	100	100
All	All	2428/3588 (68%)	2413 (99%)	15 (1%)	82	88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	135	ARG
2	D	135	ARG
2	B	619	ASN
2	D	619	ASN
3	C	619	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	112	GLN
3	C	243	GLN
2	D	18	GLN
3	C	334	GLN
2	B	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

21 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	$\# Z > 2$
10	NAG	P	1	1,10	14,14,15	0.55	0	17,19,21	1.38	2 (11%)
10	NAG	P	2	10	14,14,15	0.59	0	17,19,21	1.06	2 (11%)
10	BMA	P	3	10	11,11,12	0.71	0	15,15,17	0.92	1 (6%)
10	NAG	Q	1	1,10	14,14,15	0.31	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	Q	2	10	14,14,15	0.26	0	17,19,21	0.60	0
10	BMA	Q	3	10	11,11,12	0.95	0	15,15,17	0.74	0
11	NAG	R	1	11	14,14,15	5.25	1 (7%)	17,19,21	3.07	3 (17%)
11	NAG	R	2	11	14,14,15	0.30	0	17,19,21	0.57	0
11	NAG	S	1	2,11	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
11	NAG	S	2	11	14,14,15	0.46	0	17,19,21	0.63	1 (5%)
10	NAG	T	1	3,10	14,14,15	0.74	1 (7%)	17,19,21	2.07	4 (23%)
10	NAG	T	2	10	14,14,15	0.33	0	17,19,21	0.64	0
10	BMA	T	3	10	11,11,12	0.75	0	15,15,17	0.83	0
10	NAG	U	1	3,10	14,14,15	0.47	0	17,19,21	0.37	0
10	NAG	U	2	10	14,14,15	0.50	0	17,19,21	1.08	1 (5%)
10	BMA	U	3	10	11,11,12	0.79	0	15,15,17	0.79	0
10	NAG	V	1	3,10	14,14,15	0.30	0	17,19,21	0.67	0
10	NAG	V	2	10	14,14,15	1.30	2 (14%)	17,19,21	0.50	0
10	BMA	V	3	10	11,11,12	0.77	0	15,15,17	0.85	0
11	NAG	W	1	2,11	14,14,15	0.98	1 (7%)	17,19,21	2.53	4 (23%)
11	NAG	W	2	11	14,14,15	0.43	0	17,19,21	0.43	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
10	NAG	P	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	P	2	10	-	4/6/23/26	0/1/1/1
10	BMA	P	3	10	-	0/2/19/22	0/1/1/1
10	NAG	Q	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Q	3	10	-	1/2/19/22	0/1/1/1
11	NAG	R	1	11	-	5/6/23/26	0/1/1/1
11	NAG	R	2	11	-	4/6/23/26	0/1/1/1
11	NAG	S	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	2/6/23/26	0/1/1/1
10	NAG	T	1	3,10	-	3/6/23/26	0/1/1/1
10	NAG	T	2	10	-	2/6/23/26	0/1/1/1
10	BMA	T	3	10	-	0/2/19/22	0/1/1/1
10	NAG	U	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	U	3	10	-	1/2/19/22	0/1/1/1
10	NAG	V	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
11	NAG	W	1	2,11	-	5/6/23/26	0/1/1/1
11	NAG	W	2	11	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	1	NAG	C1-C2	19.56	1.79	1.52
10	V	2	NAG	O5-C1	3.58	1.49	1.43
10	V	2	NAG	C1-C2	3.21	1.56	1.52
10	T	1	NAG	O5-C1	-2.35	1.39	1.43
11	W	1	NAG	O5-C1	-2.34	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	1	NAG	O5-C1-C2	-9.23	97.00	111.29
11	W	1	NAG	C2-N2-C7	8.14	133.81	122.90
11	R	1	NAG	C1-O5-C5	7.87	122.73	112.19
10	T	1	NAG	C1-O5-C5	5.23	119.19	112.19
11	W	1	NAG	C1-C2-N2	4.39	117.35	110.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	1	NAG	C1-C2-N2-C7
11	R	1	NAG	C8-C7-N2-C2
11	R	1	NAG	O7-C7-N2-C2
11	R	2	NAG	C3-C2-N2-C7
10	P	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 15 short contacts:

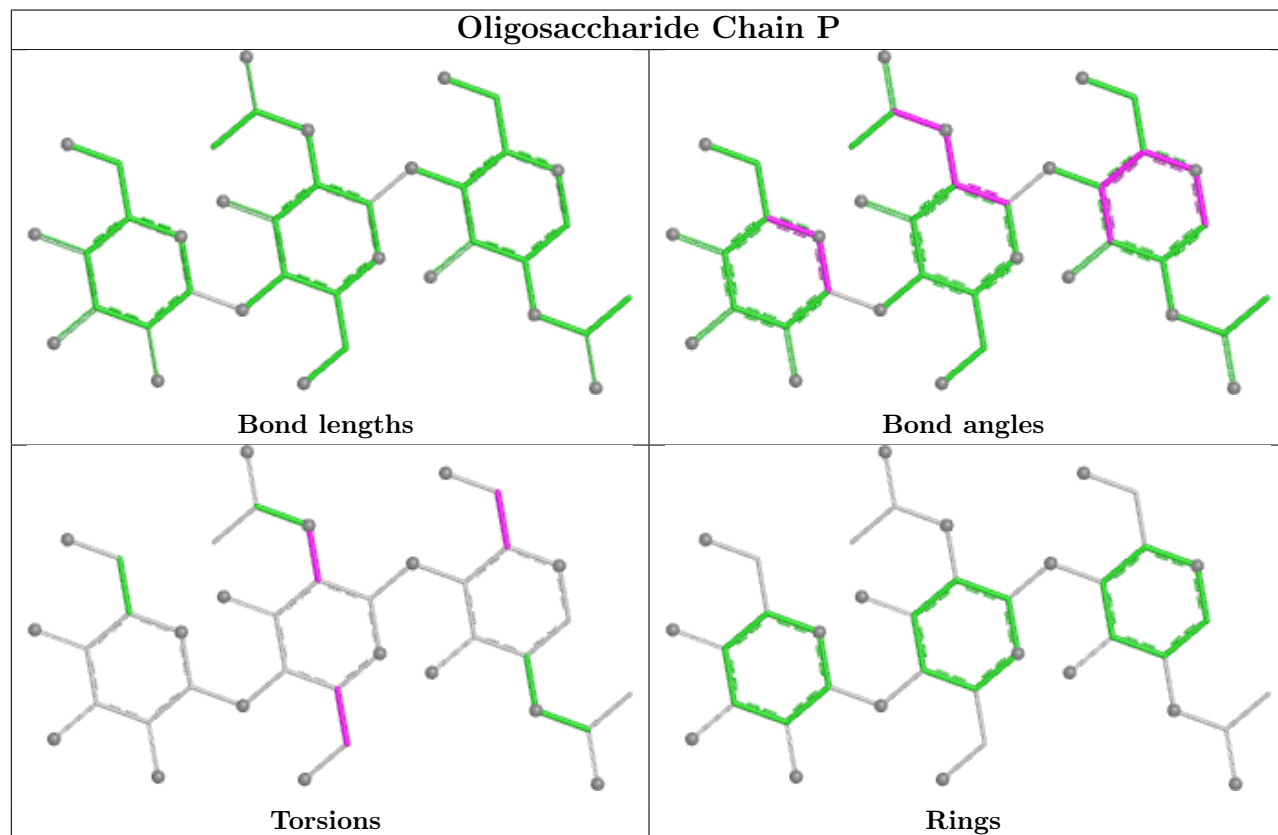
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	R	1	NAG	11	0

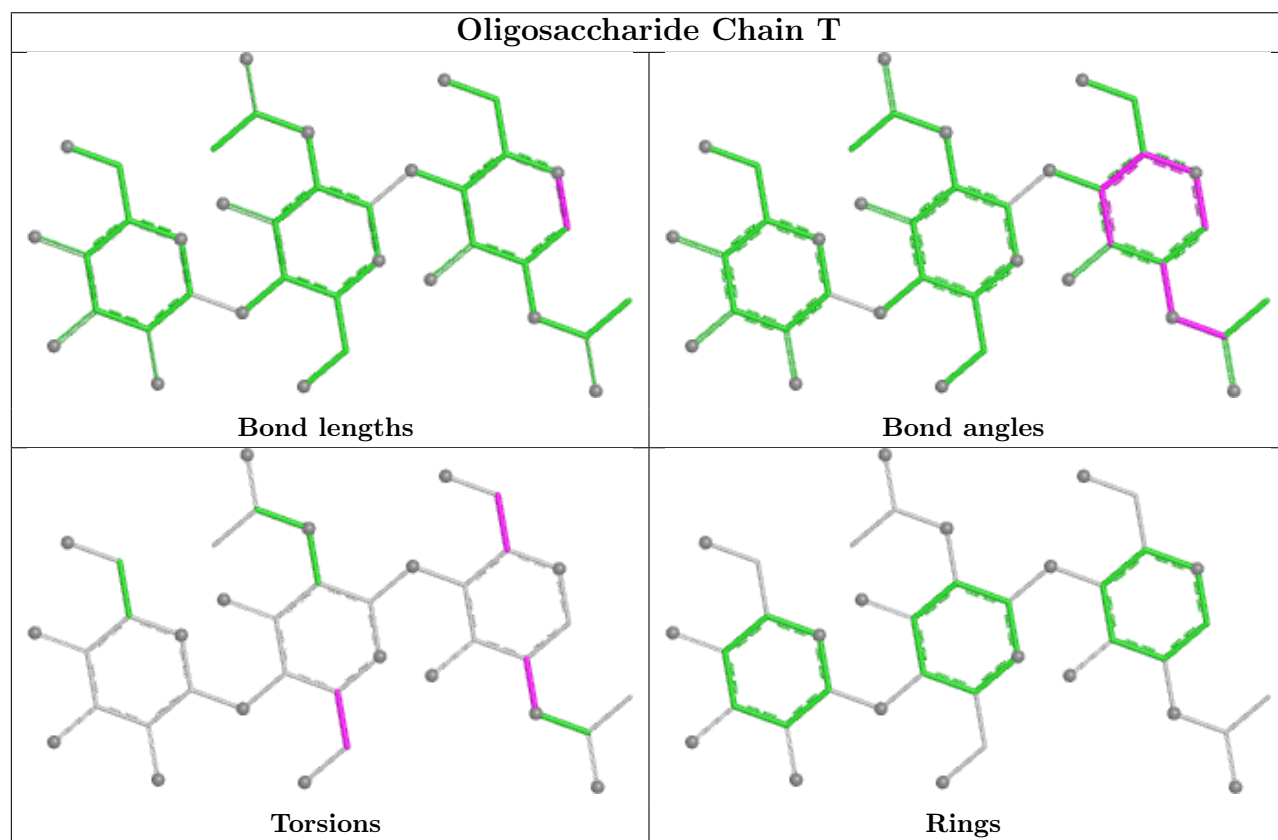
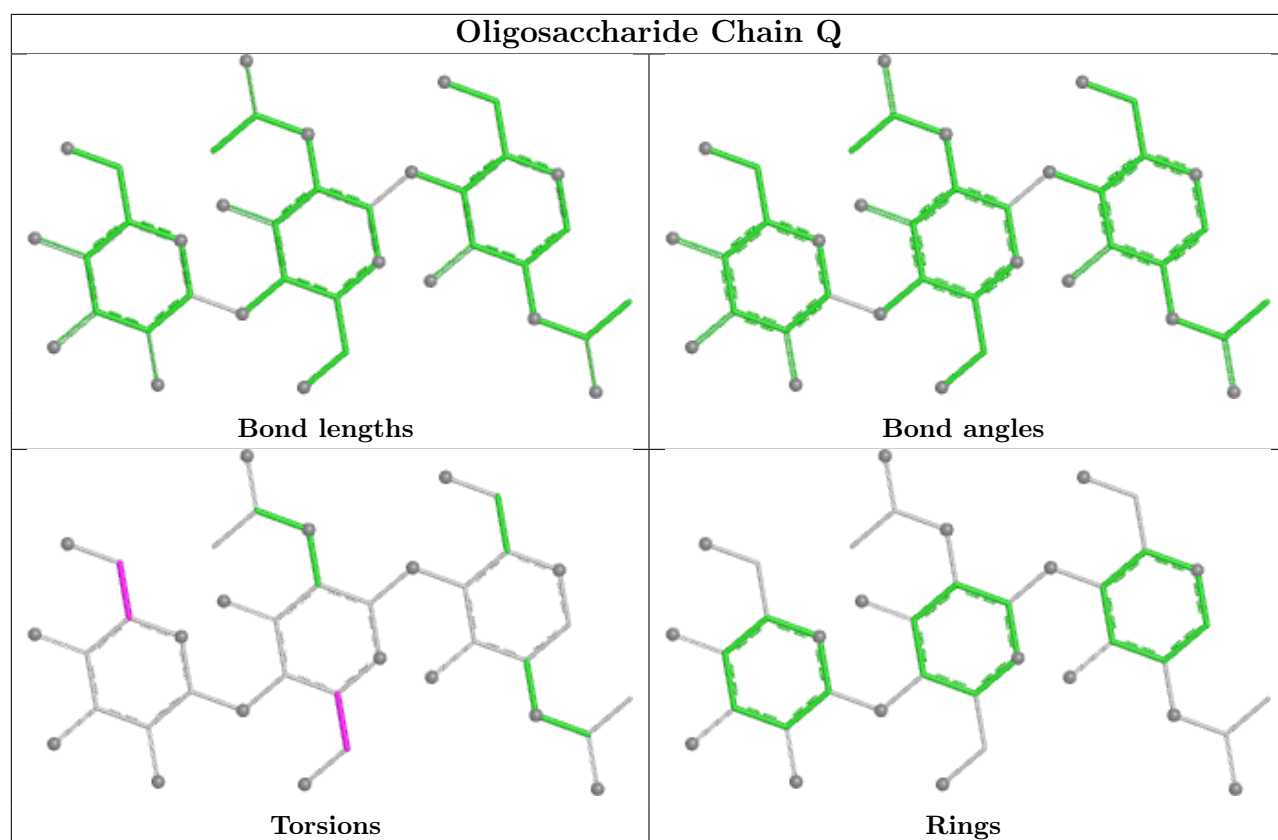
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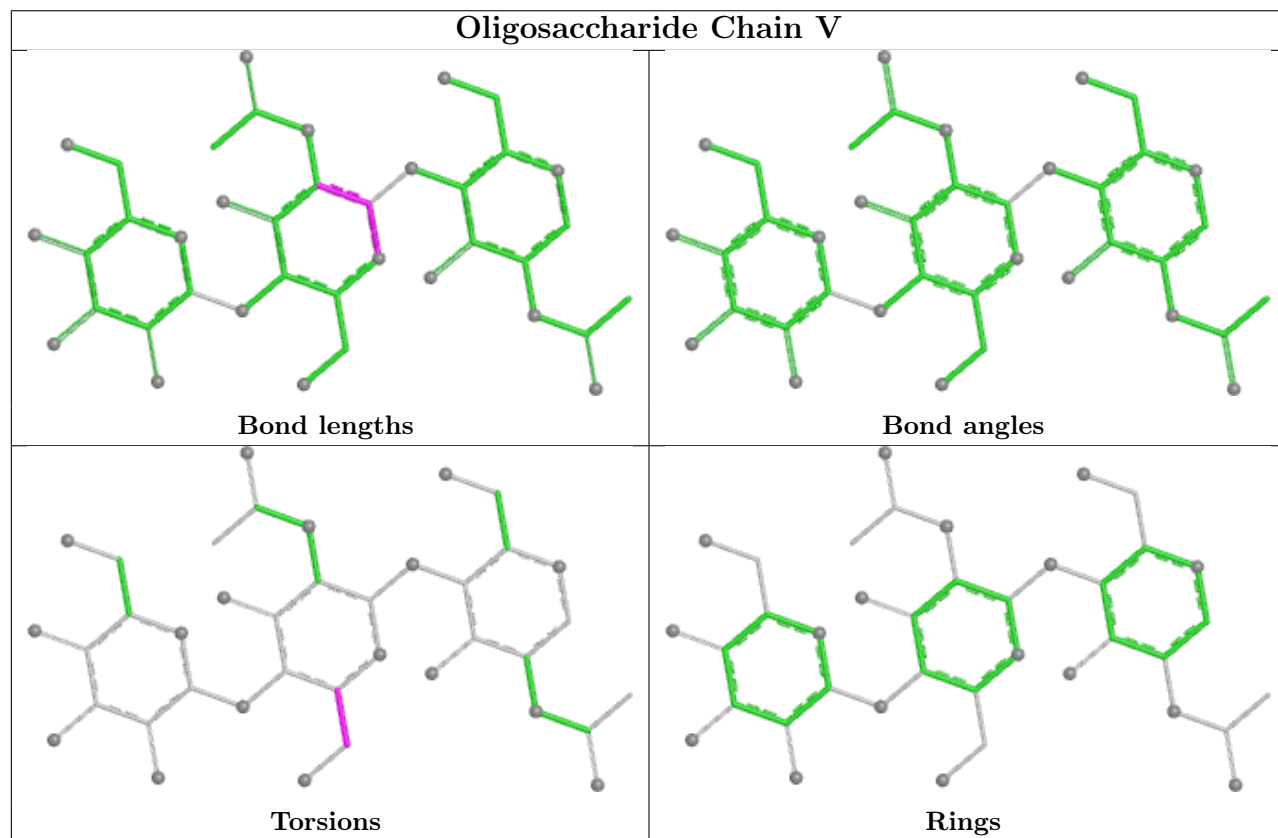
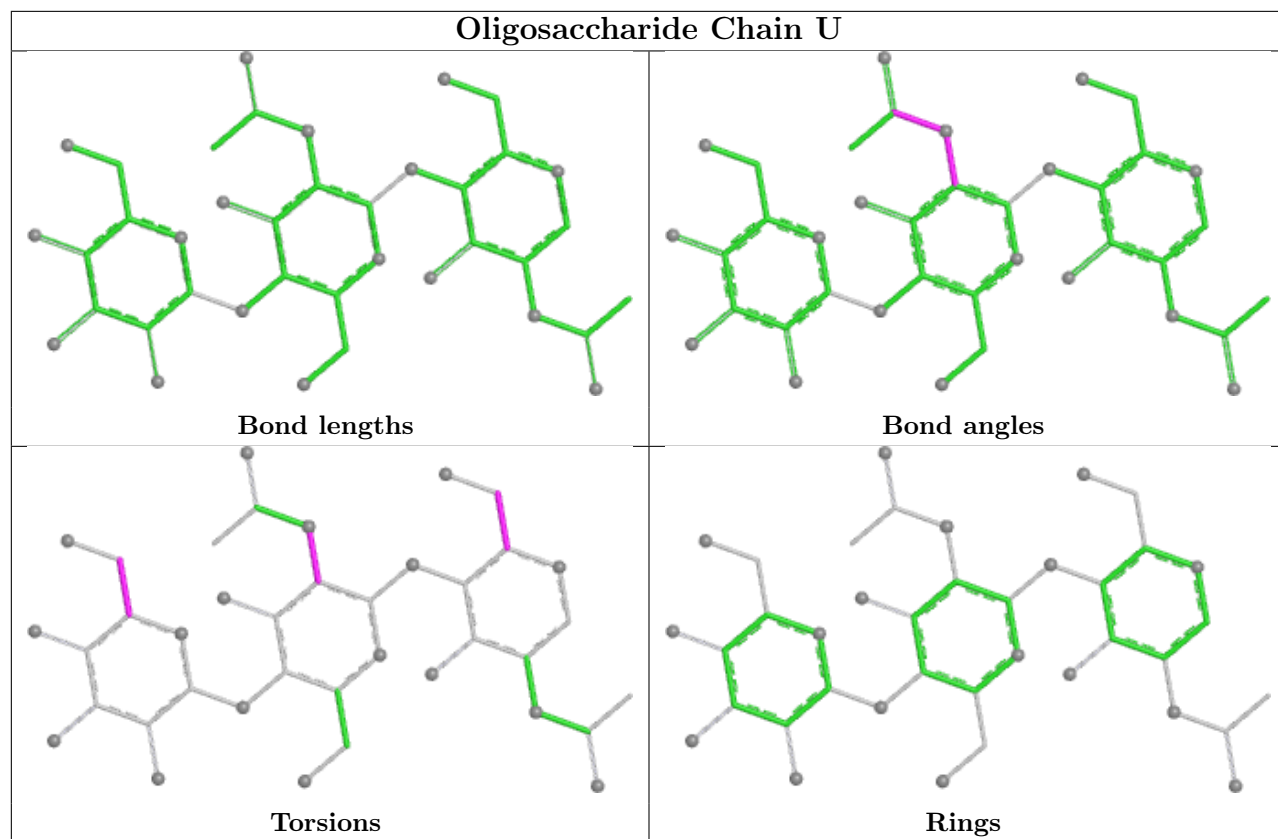
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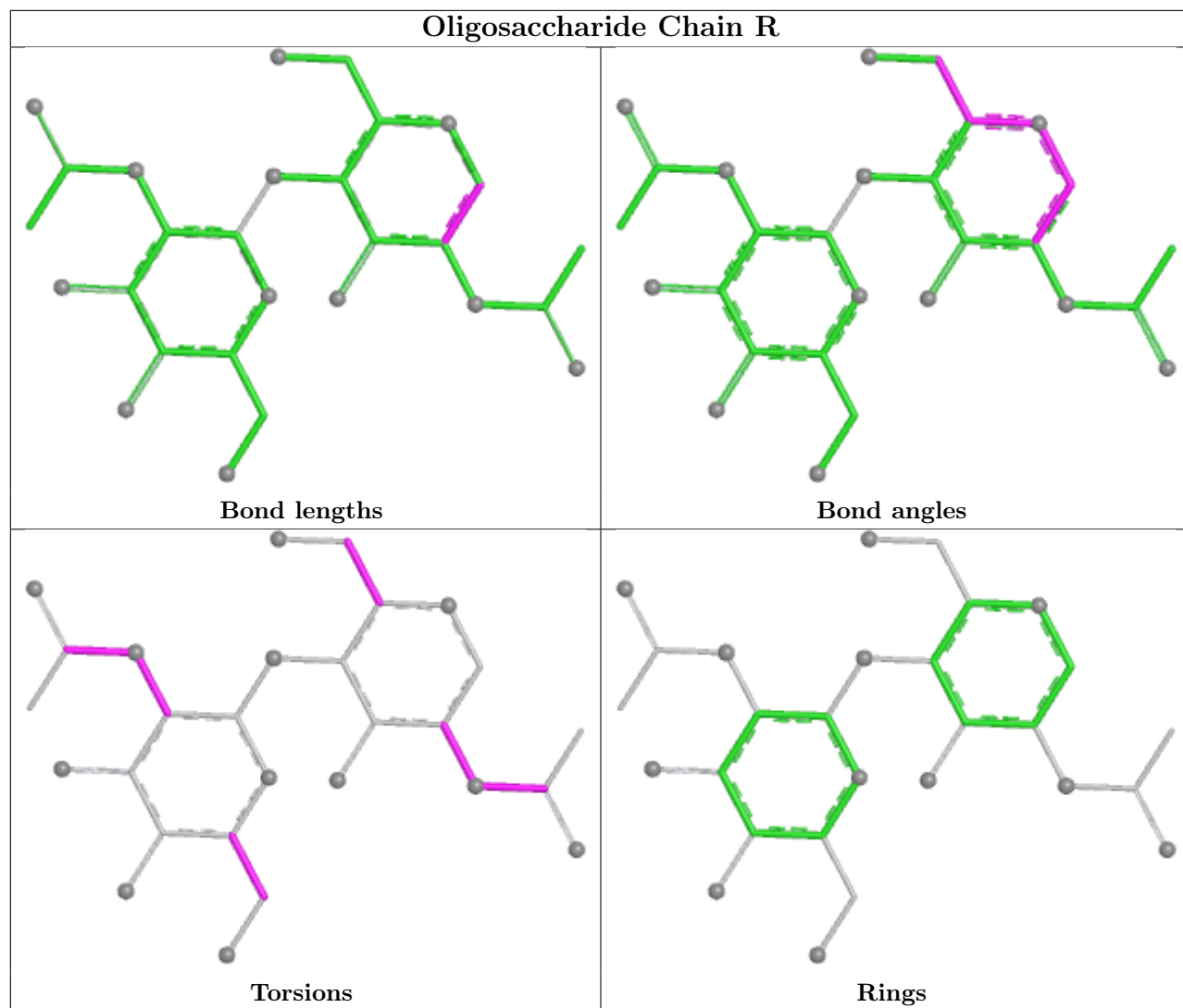
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	R	2	NAG	2	0
10	U	1	NAG	2	0

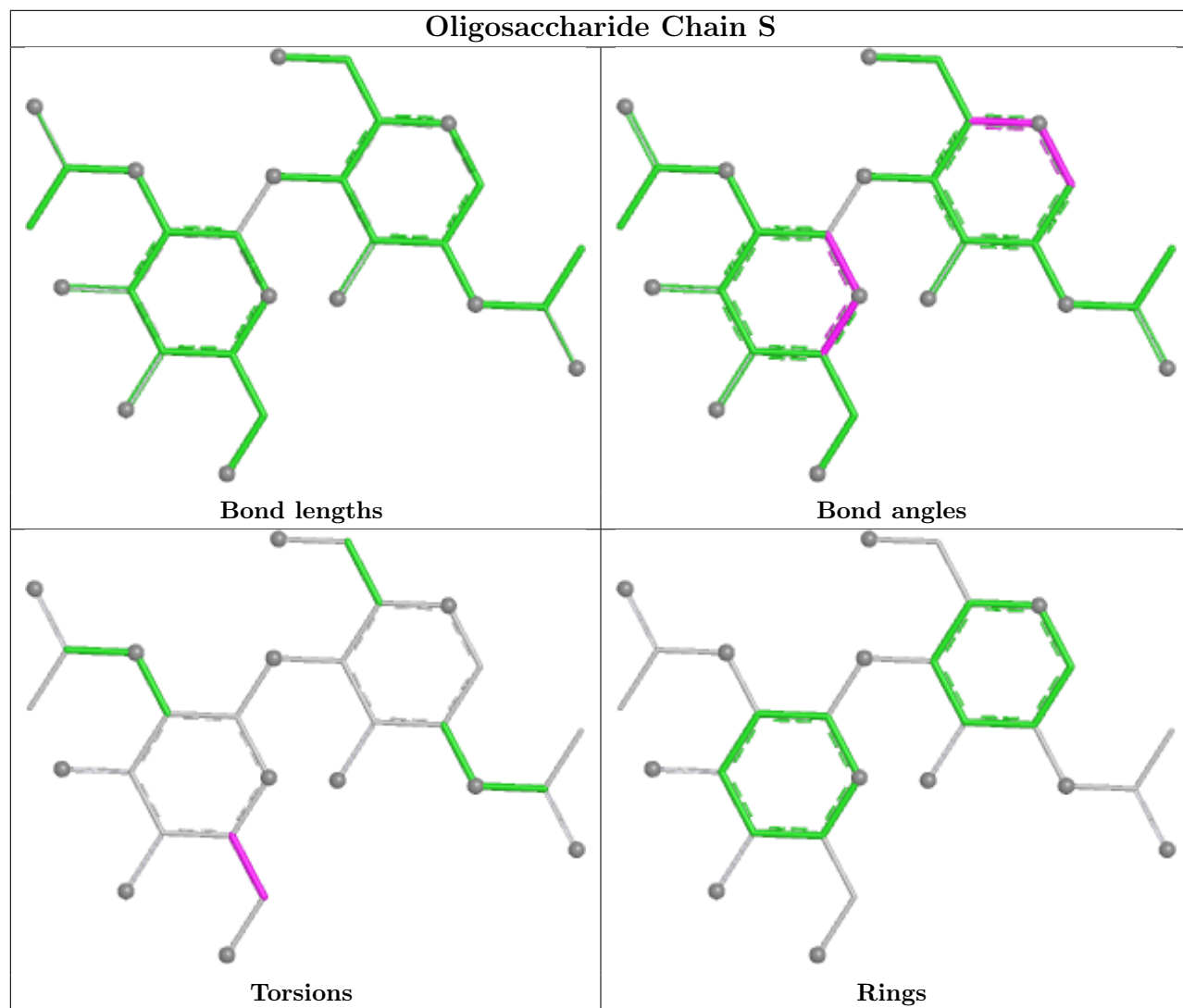
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

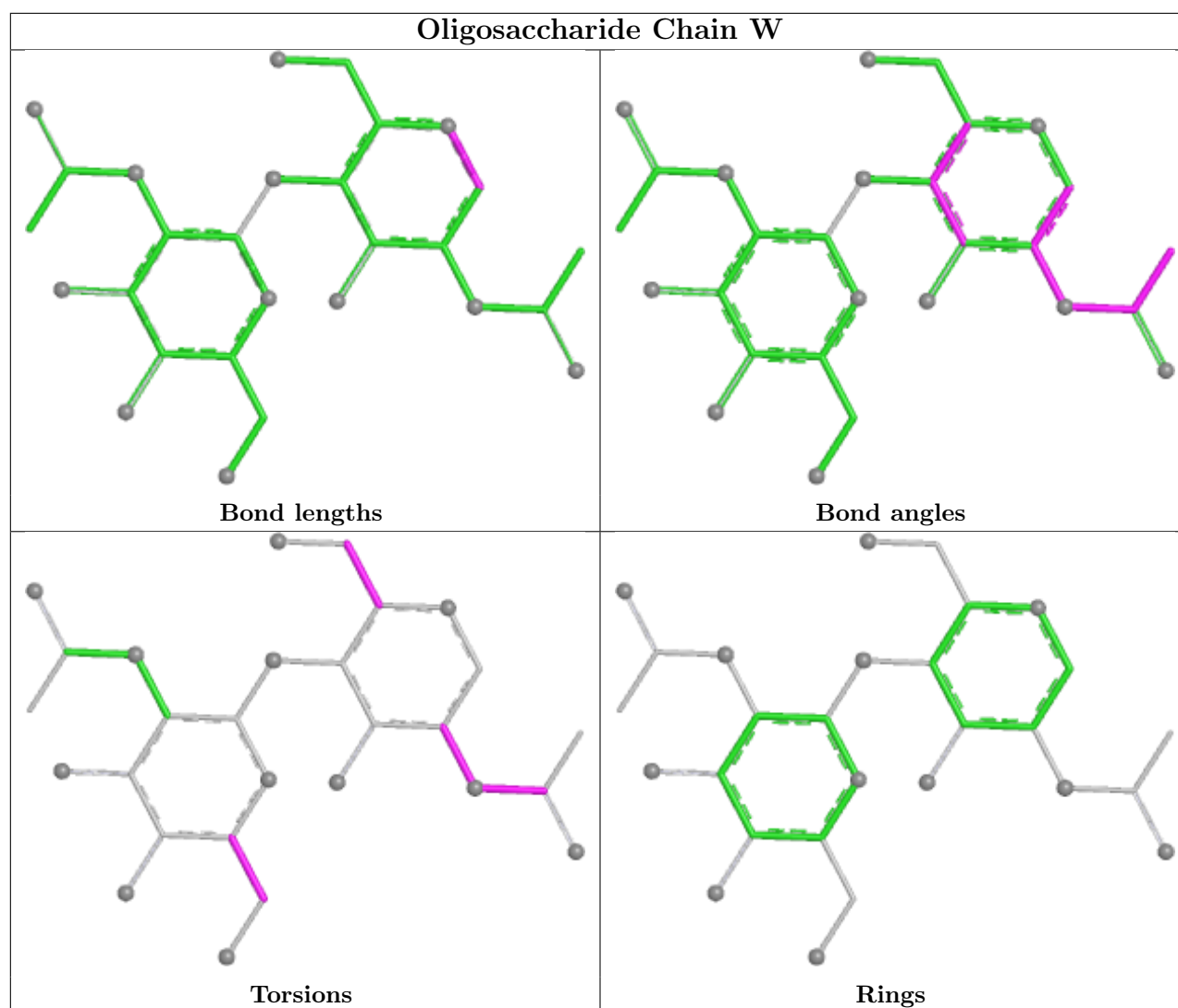












5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
12	ZK1	C	901	-	29,29,29	3.31	10 (34%)	45,45,45	1.71	11 (24%)
12	ZK1	A	901	-	29,29,29	3.33	10 (34%)	45,45,45	1.61	9 (20%)
12	ZK1	D	901	-	29,29,29	3.29	10 (34%)	45,45,45	1.70	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	A	902	1	14,14,15	0.59	0	17,19,21	0.50	0
13	NAG	B	902	2	14,14,15	0.32	0	17,19,21	0.51	0
13	NAG	D	902	2	14,14,15	0.34	0	17,19,21	0.50	0
12	ZK1	B	901	-	29,29,29	3.33	10 (34%)	45,45,45	1.76	12 (26%)

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
12	ZK1	C	901	-	-	4/13/23/23	0/3/3/3
12	ZK1	A	901	-	-	5/13/23/23	0/3/3/3
12	ZK1	D	901	-	-	4/13/23/23	0/3/3/3
13	NAG	A	902	1	-	2/6/23/26	0/1/1/1
13	NAG	B	902	2	-	0/6/23/26	0/1/1/1
13	NAG	D	902	2	-	0/6/23/26	0/1/1/1
12	ZK1	B	901	-	-	4/13/23/23	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	901	ZK1	CAU-CAT	-10.18	1.39	1.53
12	B	901	ZK1	CAU-CAT	-10.08	1.39	1.53
12	D	901	ZK1	CAU-CAT	-10.04	1.39	1.53
12	C	901	ZK1	CAU-CAT	-10.02	1.39	1.53
12	C	901	ZK1	OAA-CAT	8.89	1.40	1.23

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	901	ZK1	CAN-NAX-CAM	4.94	122.67	111.57
12	D	901	ZK1	CAN-NAX-CAM	4.65	122.03	111.57
12	B	901	ZK1	CAN-NAX-CAM	4.07	120.71	111.57
12	A	901	ZK1	CAI-CAR-NAX	-3.90	116.91	122.59
12	B	901	ZK1	CAI-CAR-NAX	-3.84	116.99	122.59

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

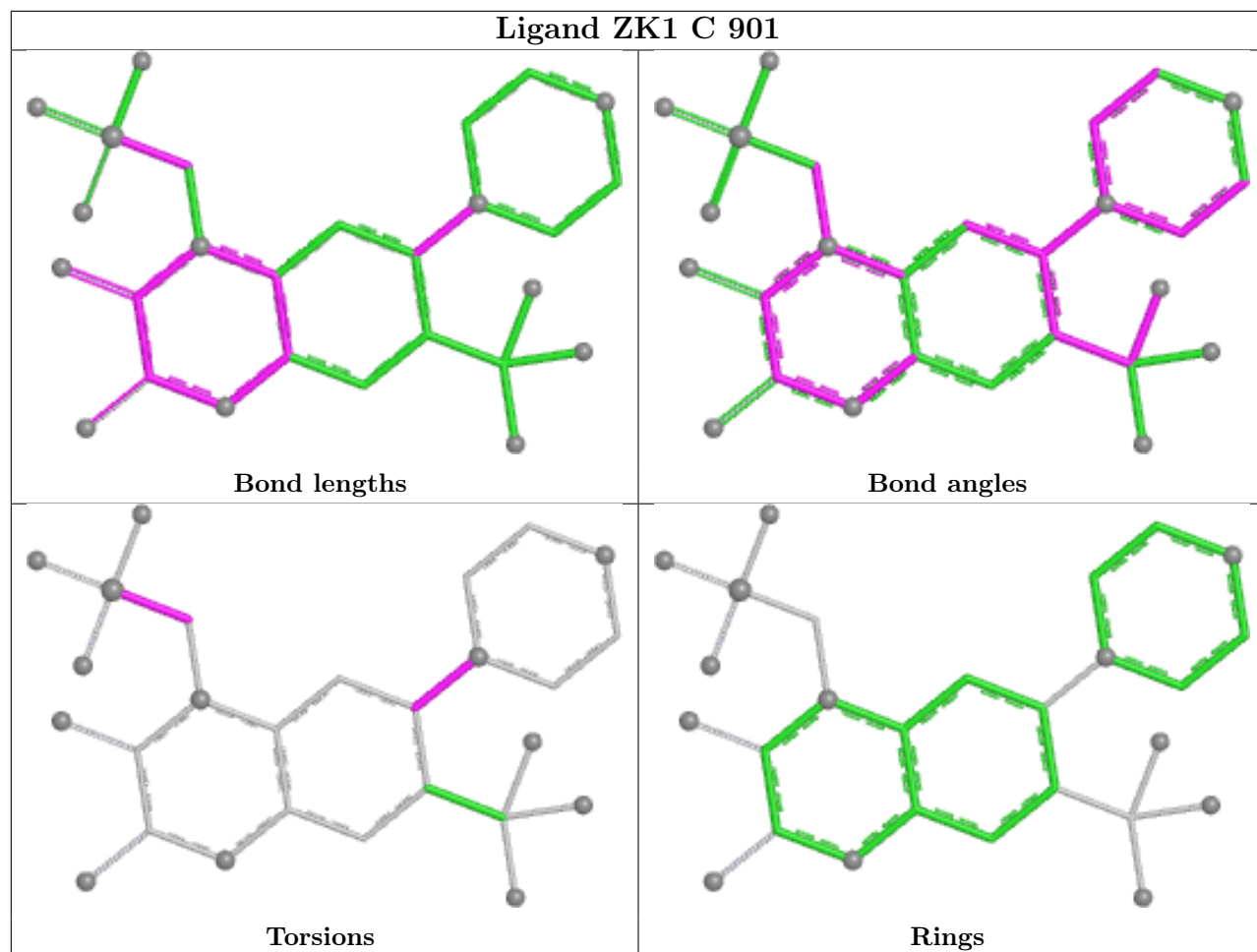
Mol	Chain	Res	Type	Atoms
12	A	901	ZK1	NAY-CAO-PBA-OAC
12	A	901	ZK1	NAY-CAO-PBA-OAE
12	B	901	ZK1	NAY-CAO-PBA-OAD
12	B	901	ZK1	NAY-CAO-PBA-OAE
12	C	901	ZK1	NAY-CAO-PBA-OAD

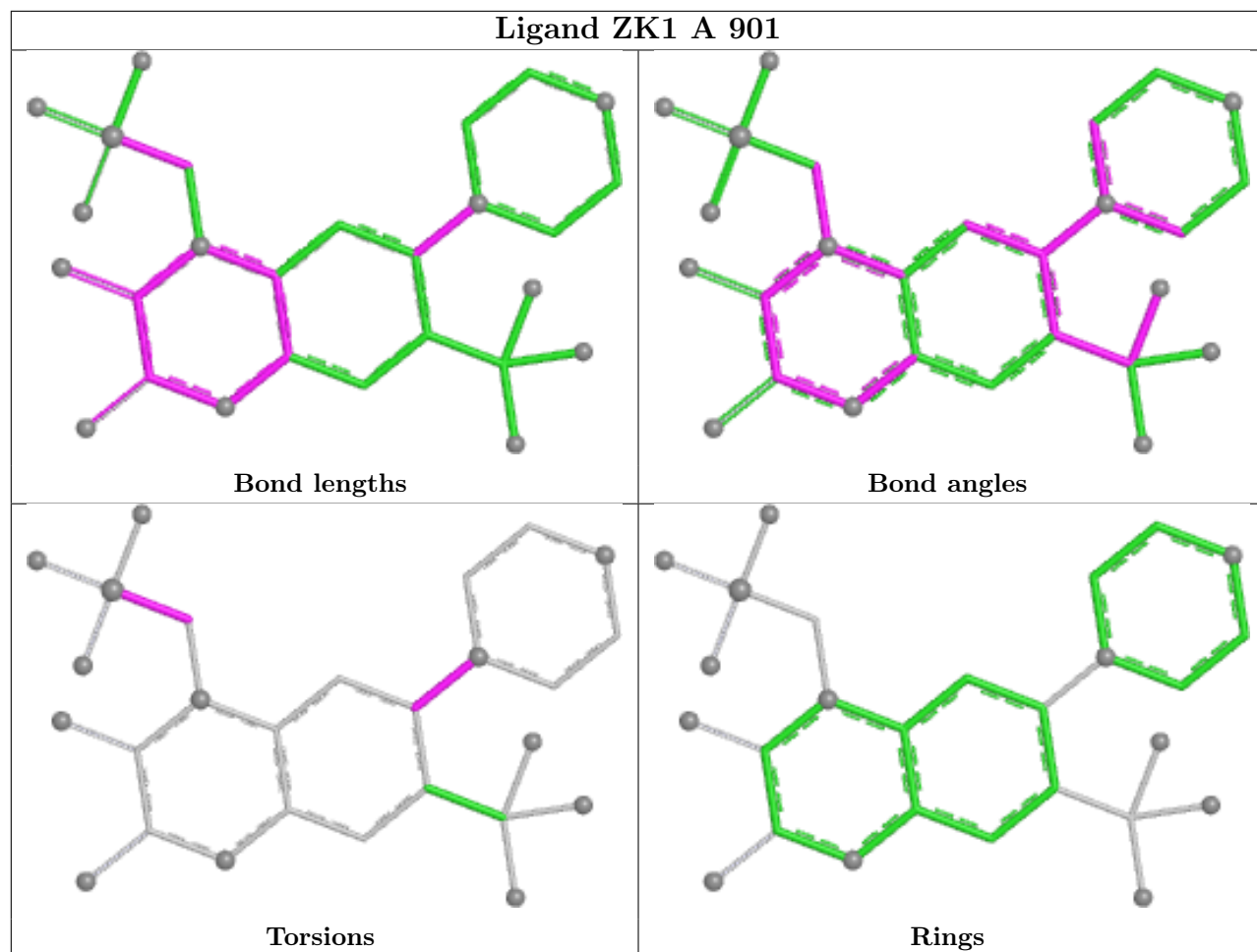
There are no ring outliers.

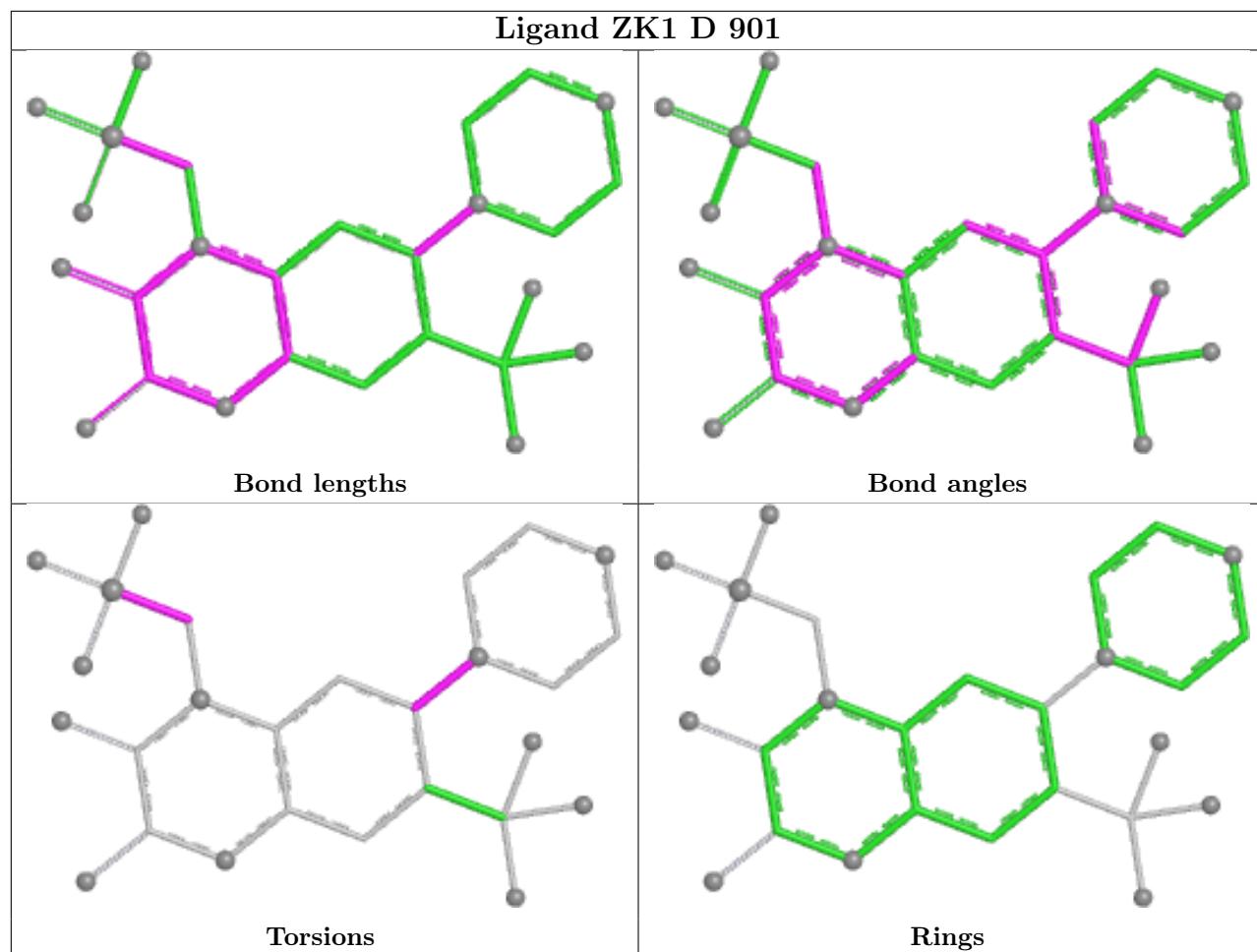
2 monomers are involved in 2 short contacts:

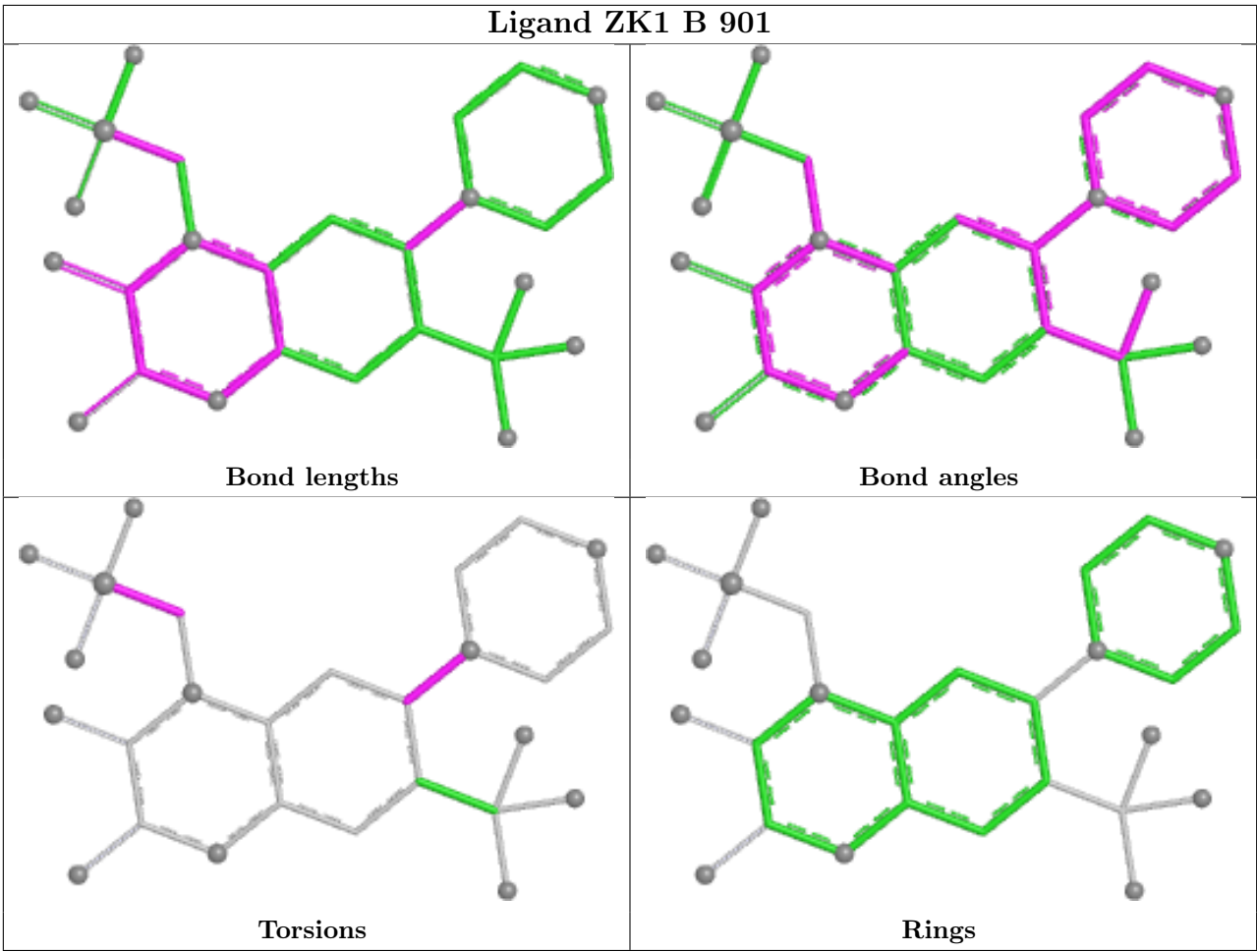
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	901	ZK1	1	0
12	D	901	ZK1	1	0

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 than 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.









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
4	E	3
4	G	3

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	20:UNK	C	21:UNK	N	14.69
1	E	54:UNK	C	55:UNK	N	14.41
1	G	54:UNK	C	55:UNK	N	14.37

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	20:UNK	C	21:UNK	N	14.16
1	E	87:UNK	C	88:UNK	N	13.08

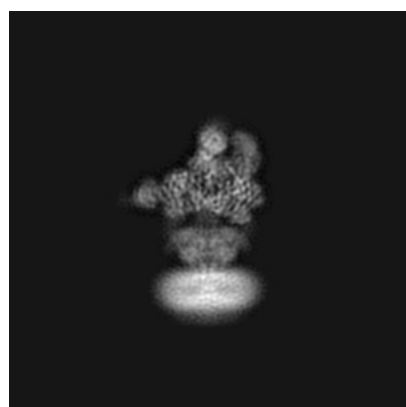
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9389. These allow visual inspection of the internal detail of the map and identification of artifacts.

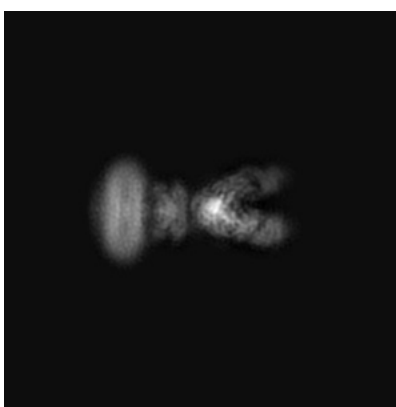
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

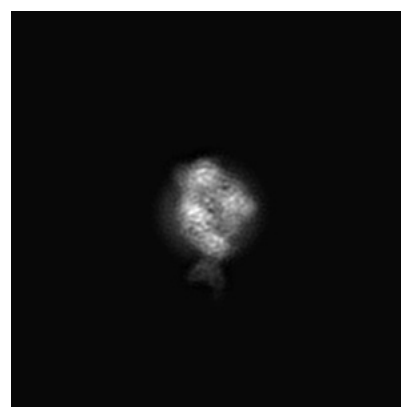
6.1.1 Primary map



X



Y



Z

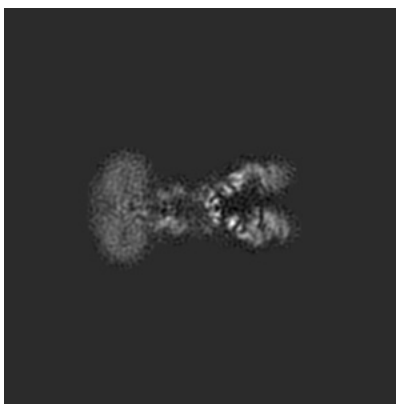
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

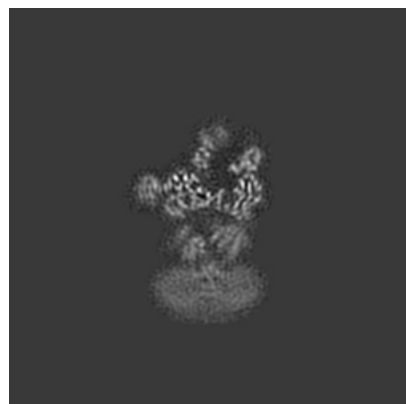


Z Index: 160

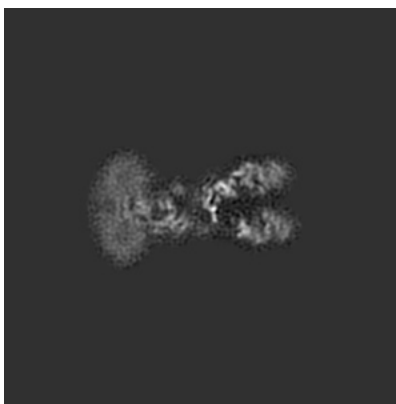
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

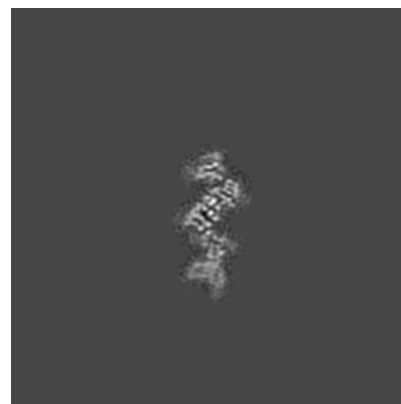
6.3.1 Primary map



X Index: 155



Y Index: 162

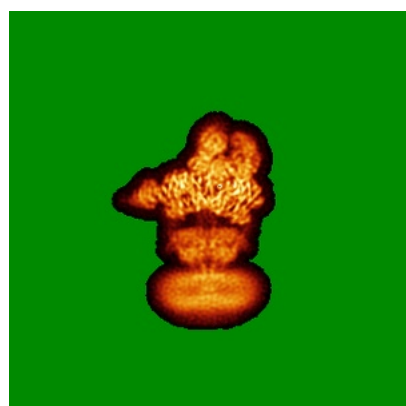


Z Index: 169

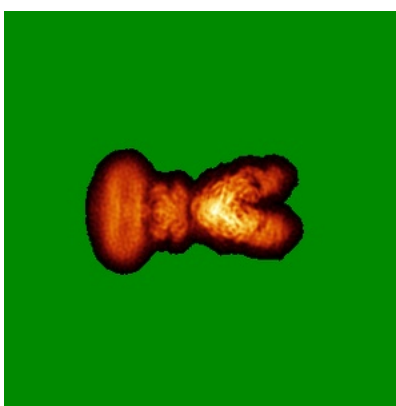
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

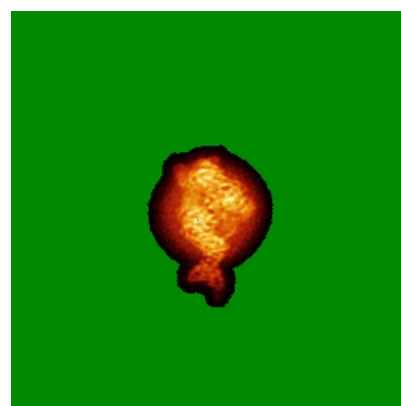
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

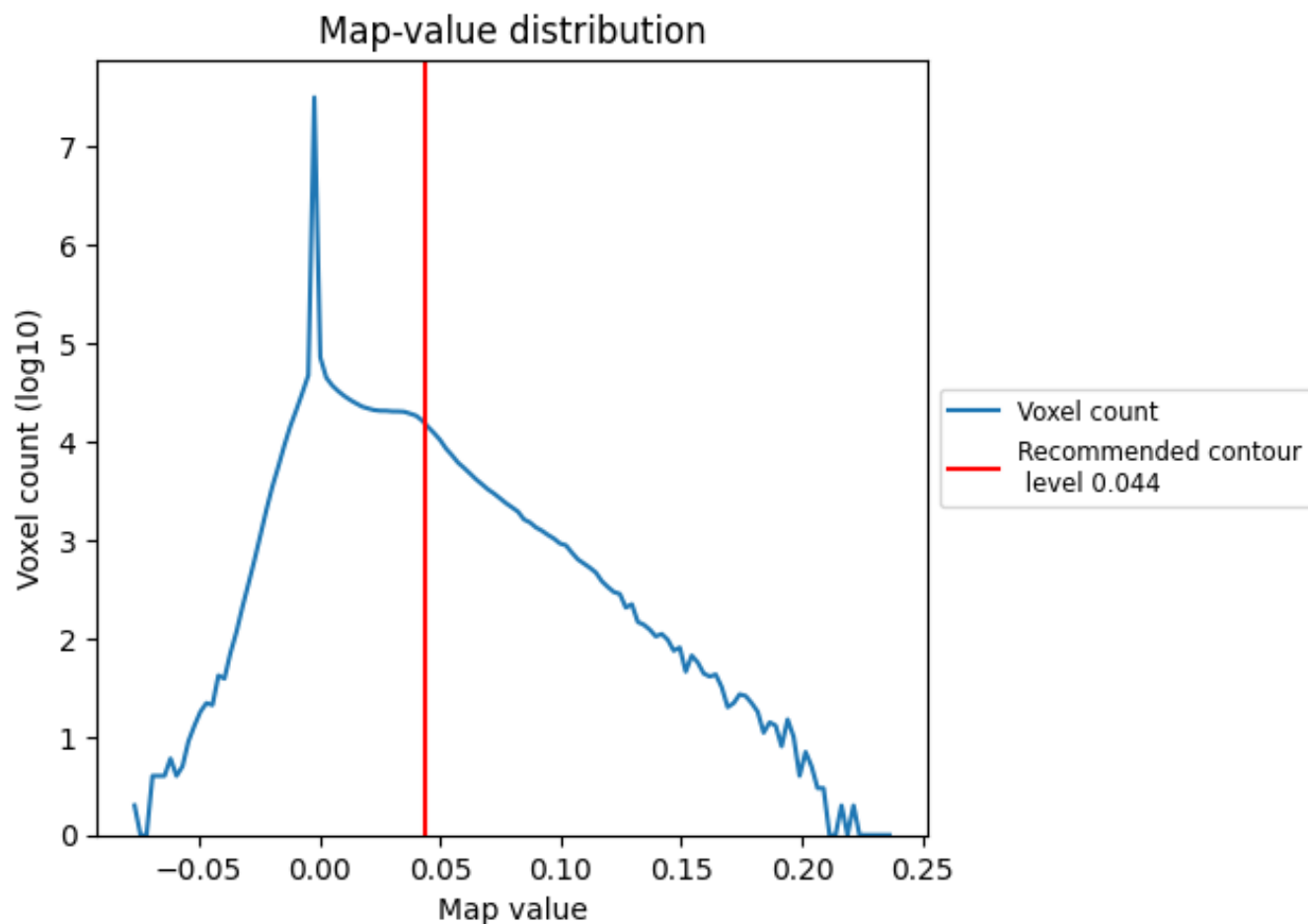
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

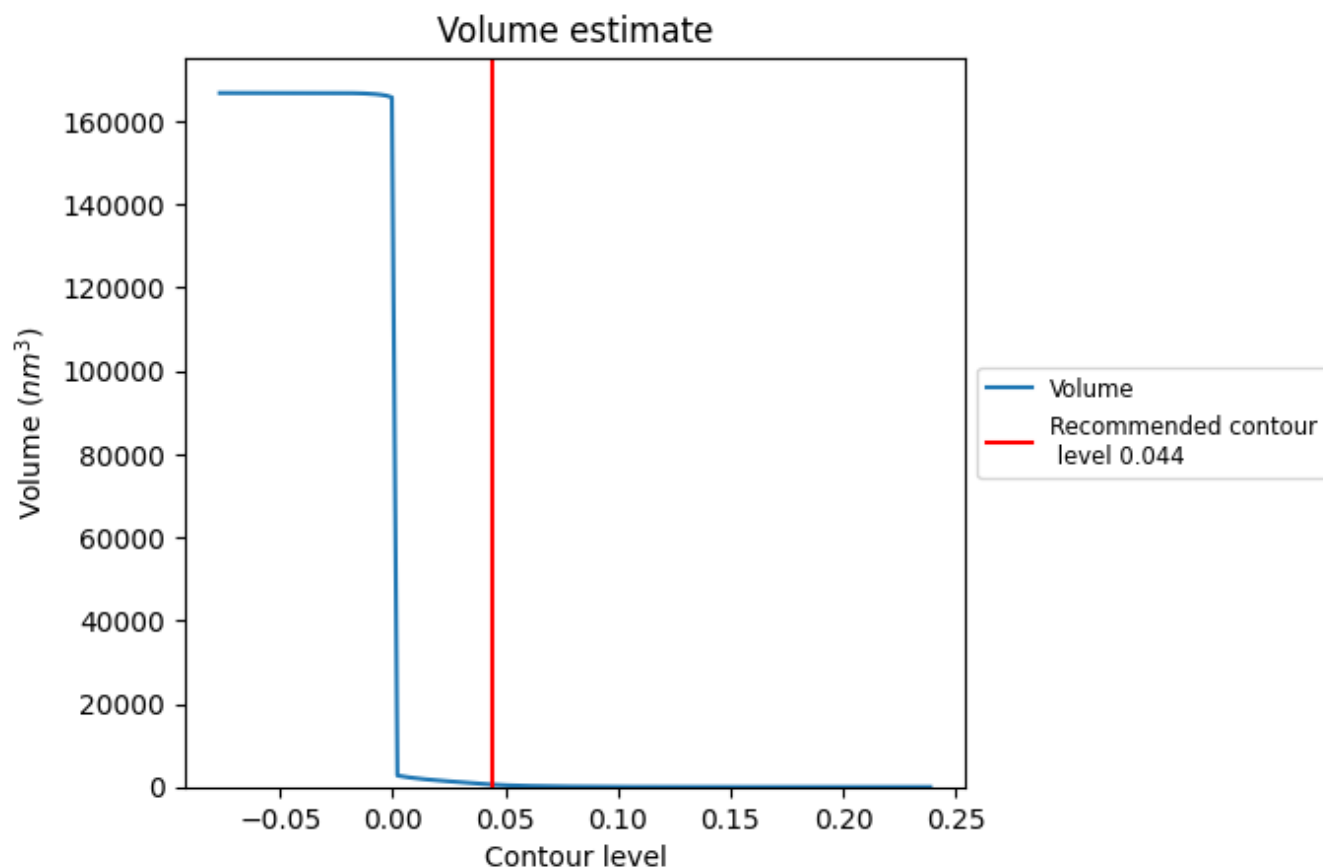
This section contains the results of statistical analysis of the map.

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.

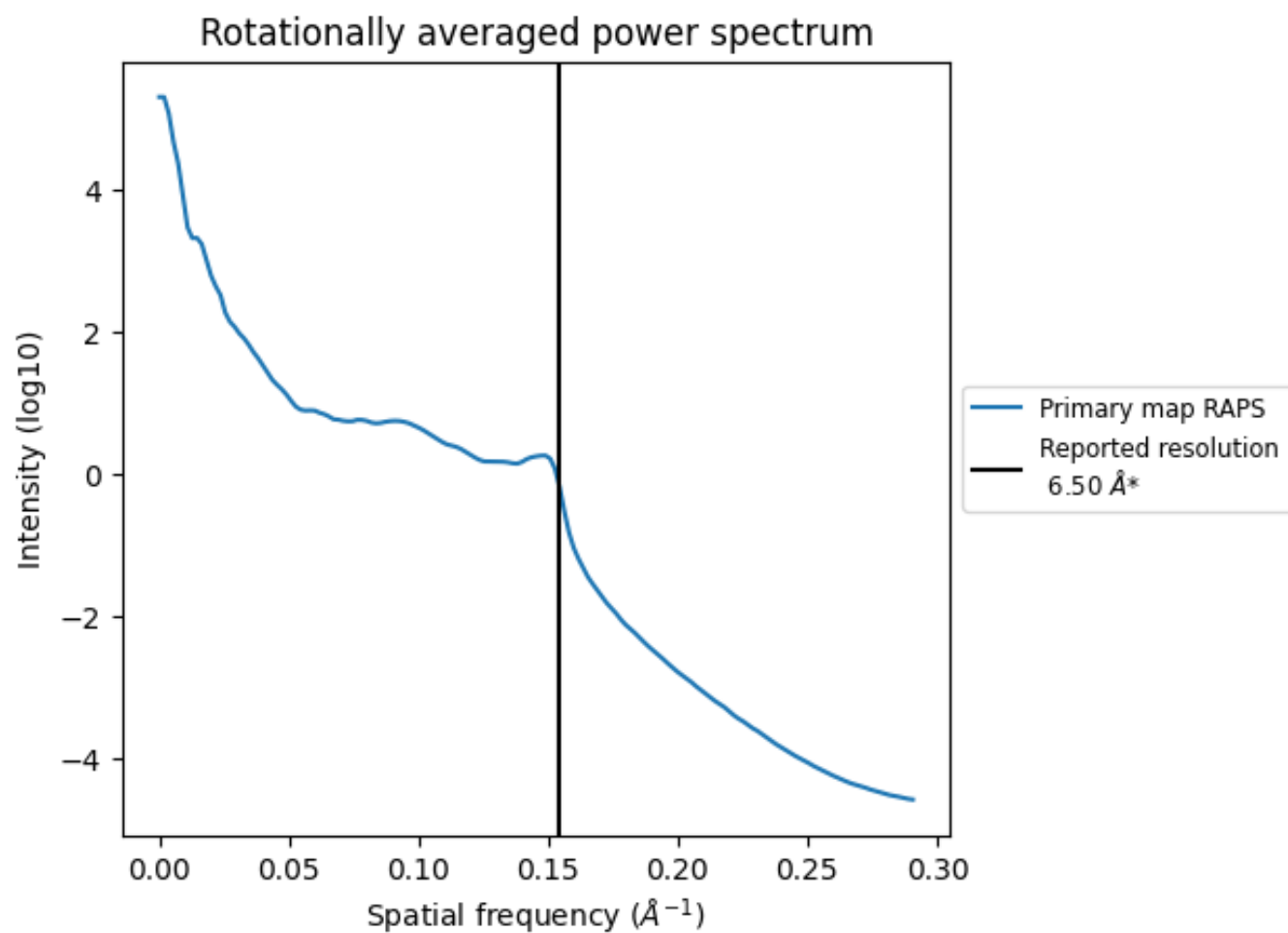
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm^3 ; this corresponds to an approximate mass of 528 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

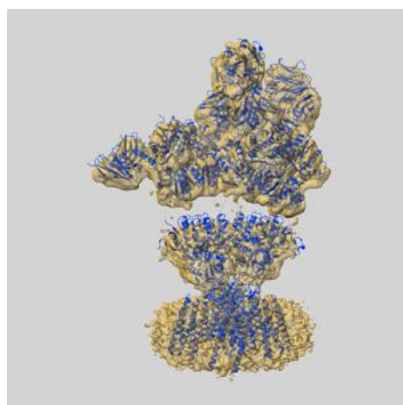
8 Fourier-Shell correlation

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

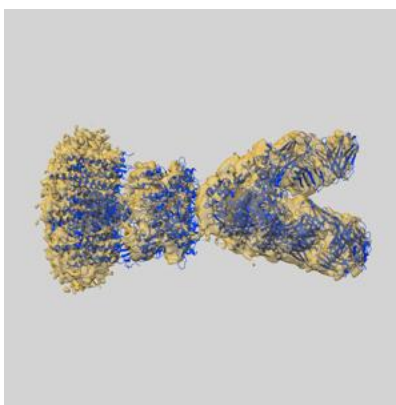
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9389 and PDB model 6NJJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

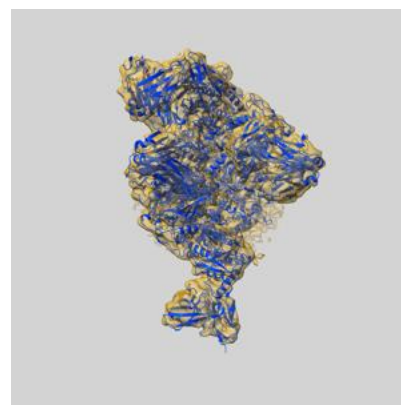
9.1 Map-model overlay [i](#)



X



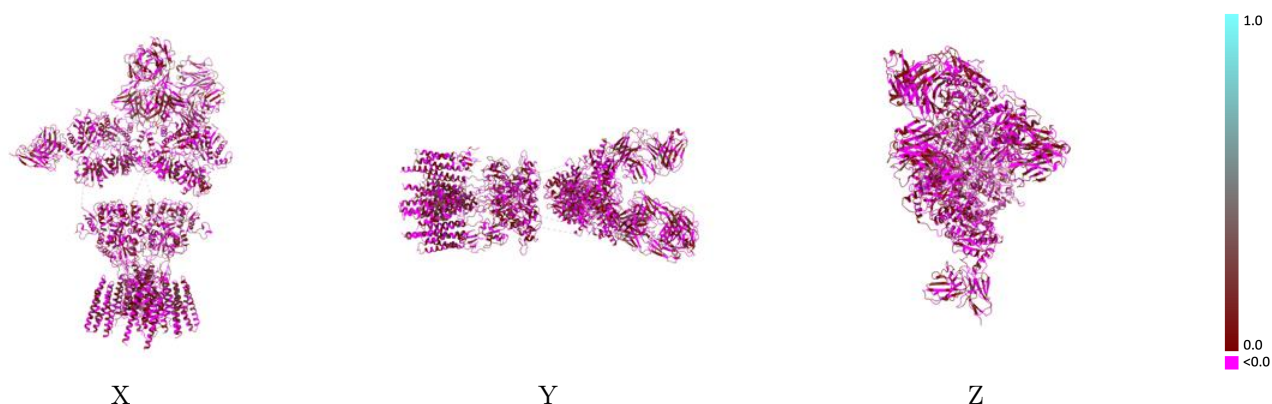
Y



Z

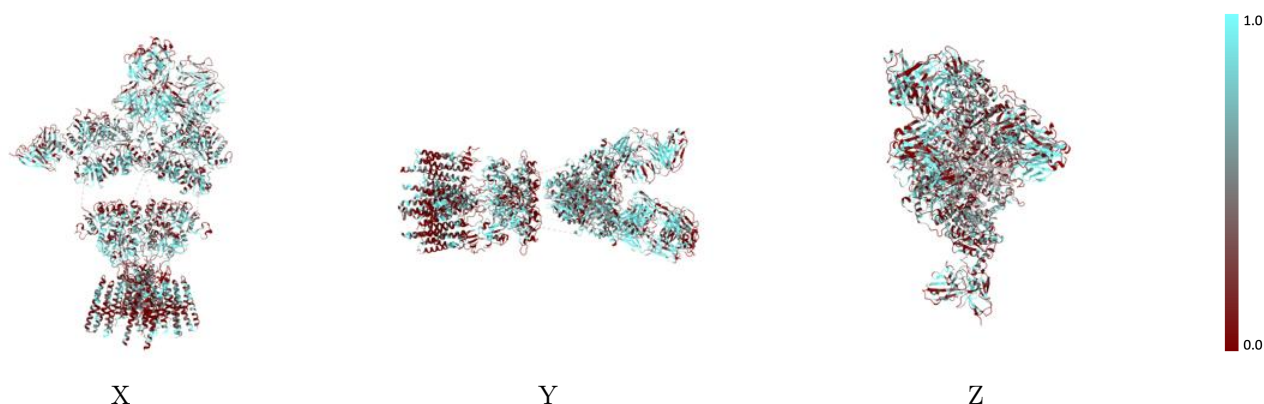
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



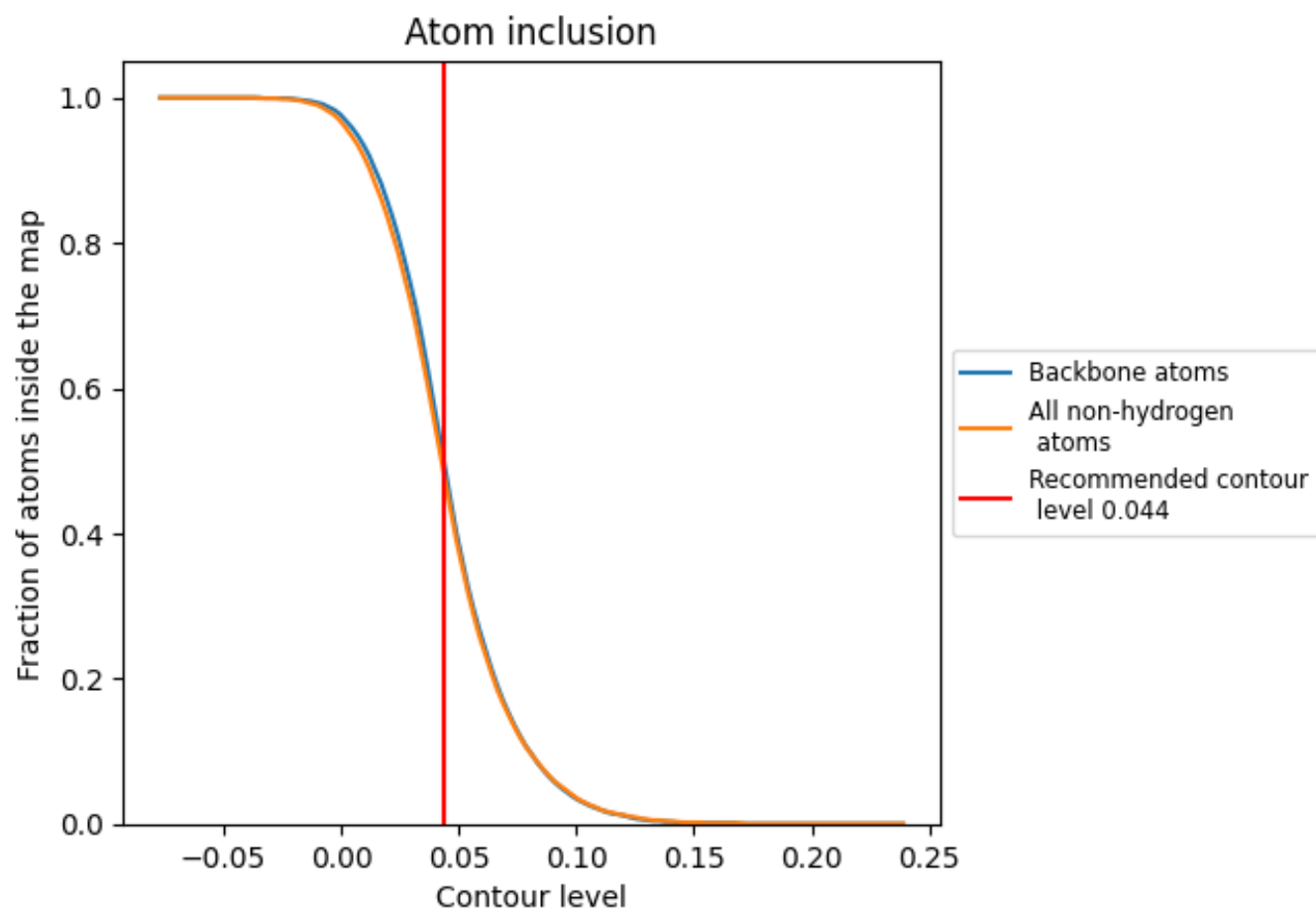
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4770	0.0120
A	0.4550	0.0060
B	0.4800	0.0090
C	0.4950	0.0150
D	0.4750	0.0070
E	0.3860	0.0200
F	0.2880	-0.0030
G	0.3950	0.0430
H	0.2700	-0.0030
I	0.4940	0.0270
J	0.4840	-0.0050
K	0.6030	0.0450
L	0.6060	0.0210
M	0.5420	0.0090
N	0.4810	0.0120
O	0.6530	0.0500
P	0.1280	-0.0620
Q	0.1030	-0.0460
R	0.6070	0.2300
S	0.8570	0.1790
T	0.2820	0.0800
U	0.3080	0.0220
V	0.5130	-0.0600
W	0.5360	-0.0050

