



# Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 06:36 PM JST

PDB ID : 8X90  
EMDB ID : EMD-38158  
Title : P/Q type calcium channel  
Authors : Yan, N.; Li, Z.; Cong, Y.; Wu, T.; Wang, T.  
Deposited on : 2023-11-29  
Resolution : 2.95 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.39



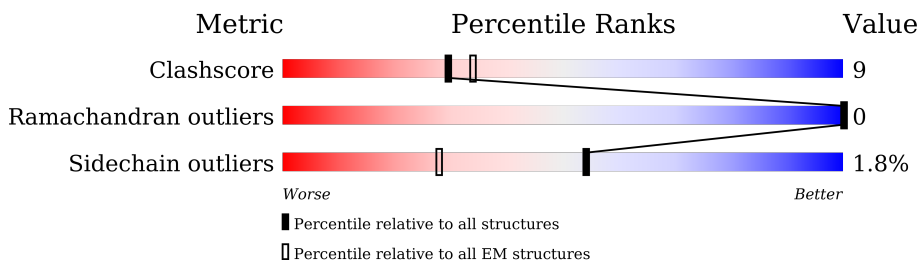
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 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  $\geq 3$ , 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	2549	 43% 10% 46%
2	B	1115	 67% 19% 14%
3	C	496	 42% 46% 20% 35%
4	D	3	 33% 67%
5	E	2	 50% 50%
5	G	2	 100%
5	H	2	 50% 50%
6	F	4	 100%



## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22122 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 Voltage-dependent P/Q-type calcium channel subunit alpha-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1377	Total	C	N	O	S	1	0
			11202	7353	1819	1950	80		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP O00555
A	-41	ALA	-	expression tag	UNP O00555
A	-40	SER	-	expression tag	UNP O00555
A	-39	TRP	-	expression tag	UNP O00555
A	-38	SER	-	expression tag	UNP O00555
A	-37	HIS	-	expression tag	UNP O00555
A	-36	PRO	-	expression tag	UNP O00555
A	-35	GLN	-	expression tag	UNP O00555
A	-34	PHE	-	expression tag	UNP O00555
A	-33	GLU	-	expression tag	UNP O00555
A	-32	LYS	-	expression tag	UNP O00555
A	-31	GLY	-	expression tag	UNP O00555
A	-30	GLY	-	expression tag	UNP O00555
A	-29	GLY	-	expression tag	UNP O00555
A	-28	ALA	-	expression tag	UNP O00555
A	-27	ARG	-	expression tag	UNP O00555
A	-26	GLY	-	expression tag	UNP O00555
A	-25	GLY	-	expression tag	UNP O00555
A	-24	SER	-	expression tag	UNP O00555
A	-23	GLY	-	expression tag	UNP O00555
A	-22	GLY	-	expression tag	UNP O00555
A	-21	GLY	-	expression tag	UNP O00555
A	-20	SER	-	expression tag	UNP O00555
A	-19	TRP	-	expression tag	UNP O00555
A	-18	SER	-	expression tag	UNP O00555
A	-17	HIS	-	expression tag	UNP O00555
A	-16	PRO	-	expression tag	UNP O00555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLN	-	expression tag	UNP O00555
A	-14	PHE	-	expression tag	UNP O00555
A	-13	GLU	-	expression tag	UNP O00555
A	-12	LYS	-	expression tag	UNP O00555
A	-11	GLY	-	expression tag	UNP O00555
A	-10	PHE	-	expression tag	UNP O00555
A	-9	ASP	-	expression tag	UNP O00555
A	-8	TYR	-	expression tag	UNP O00555
A	-7	LYS	-	expression tag	UNP O00555
A	-6	ASP	-	expression tag	UNP O00555
A	-5	ASP	-	expression tag	UNP O00555
A	-4	ASP	-	expression tag	UNP O00555
A	-3	ASP	-	expression tag	UNP O00555
A	-2	LYS	-	expression tag	UNP O00555
A	-1	GLY	-	expression tag	UNP O00555
A	0	THR	-	expression tag	UNP O00555

- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	964	Total	C	N	O	S	0	0
			7695	4879	1289	1493	34		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1104	LEU	-	expression tag	UNP P54289
B	1105	GLU	-	expression tag	UNP P54289
B	1106	HIS	-	expression tag	UNP P54289
B	1107	HIS	-	expression tag	UNP P54289
B	1108	HIS	-	expression tag	UNP P54289
B	1109	HIS	-	expression tag	UNP P54289
B	1110	HIS	-	expression tag	UNP P54289
B	1111	HIS	-	expression tag	UNP P54289
B	1112	HIS	-	expression tag	UNP P54289
B	1113	HIS	-	expression tag	UNP P54289
B	1114	HIS	-	expression tag	UNP P54289
B	1115	HIS	-	expression tag	UNP P54289

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2575	1619	467	479	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	485	LEU	-	expression tag	UNP P54284
C	486	GLU	-	expression tag	UNP P54284
C	487	HIS	-	expression tag	UNP P54284
C	488	HIS	-	expression tag	UNP P54284
C	489	HIS	-	expression tag	UNP P54284
C	490	HIS	-	expression tag	UNP P54284
C	491	HIS	-	expression tag	UNP P54284
C	492	HIS	-	expression tag	UNP P54284
C	493	HIS	-	expression tag	UNP P54284
C	494	HIS	-	expression tag	UNP P54284
C	495	HIS	-	expression tag	UNP P54284
C	496	HIS	-	expression tag	UNP P54284

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			42	24	3	15		

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



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

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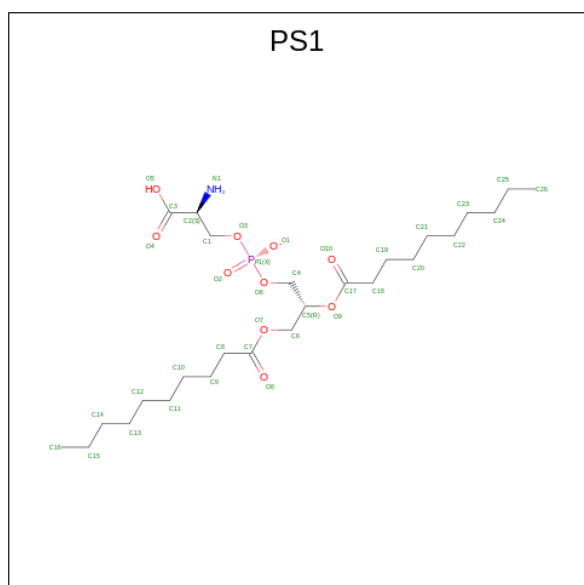
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

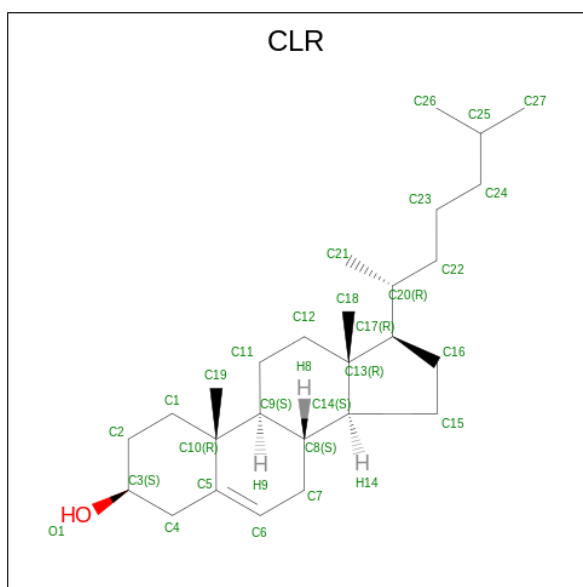
- Molecule 7 is 1,2-DIDECANOYL-SN-GLYCERO-3-[PHOSPHO-L-SERINE] (three-letter code: PS1) (formula: C<sub>26</sub>H<sub>49</sub>NO<sub>10</sub>P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			38	26	1	10	1	

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).

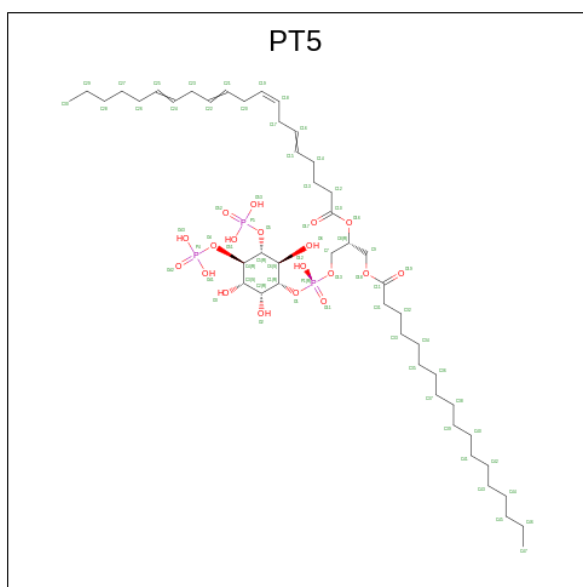




Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	

- Molecule 9 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula:  $C_{47}H_{85}O_{19}P_3$ ).





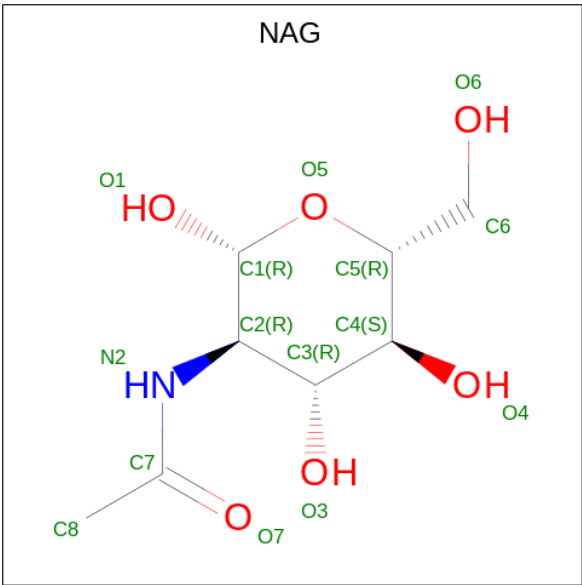
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			64	42	19	3	

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Ca	0
			1	1	
10	B	1	Total	Ca	0
			1	1	

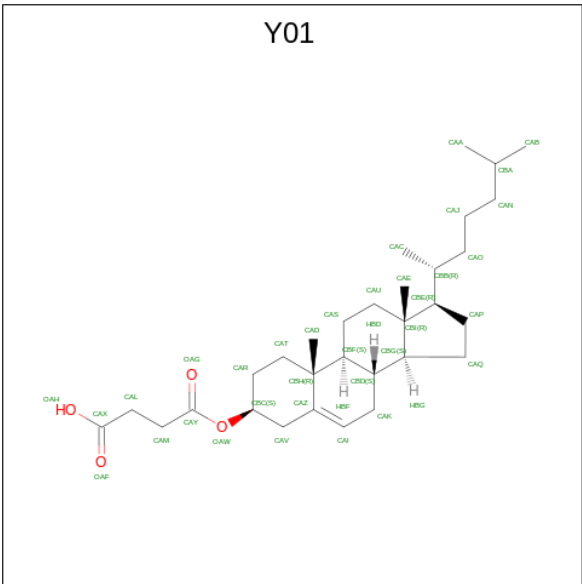
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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

- Molecule 12 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O		0
			35	31	4		

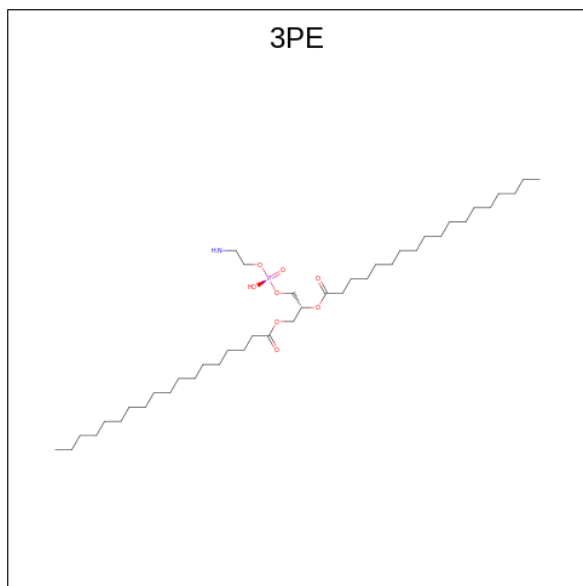
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Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			35	31	4	
12	A	1	Total	C	O	0
			35	31	4	

- Molecule 13 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
13	A	1	Total	C	N	O	P	0
			51	41	1	8	1	



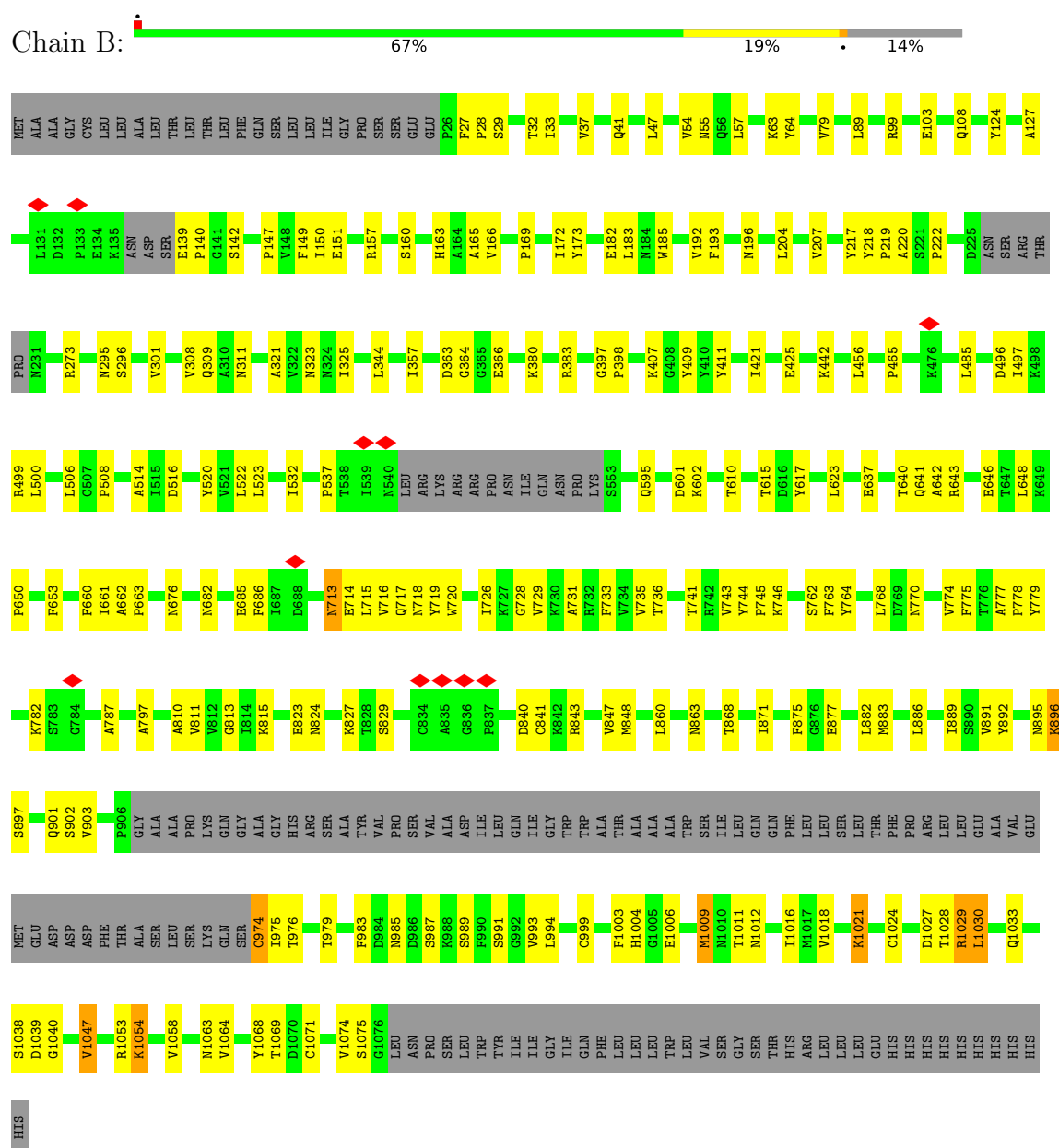




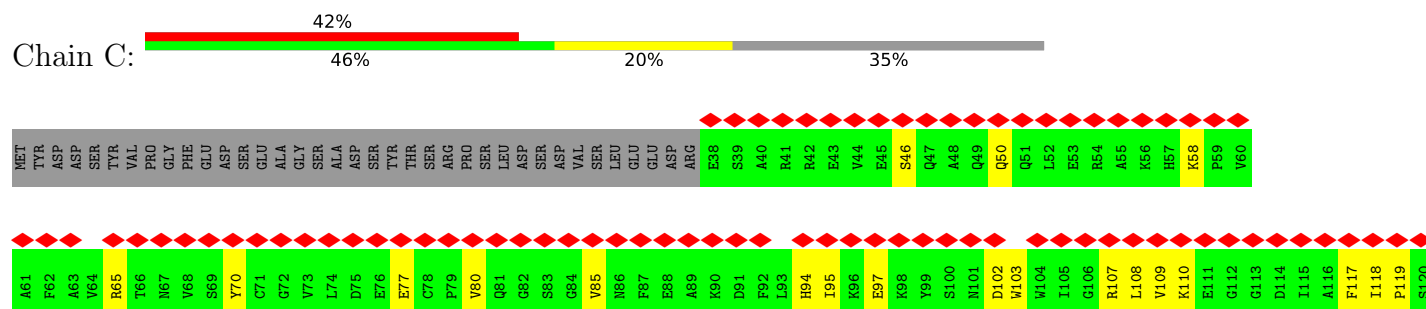




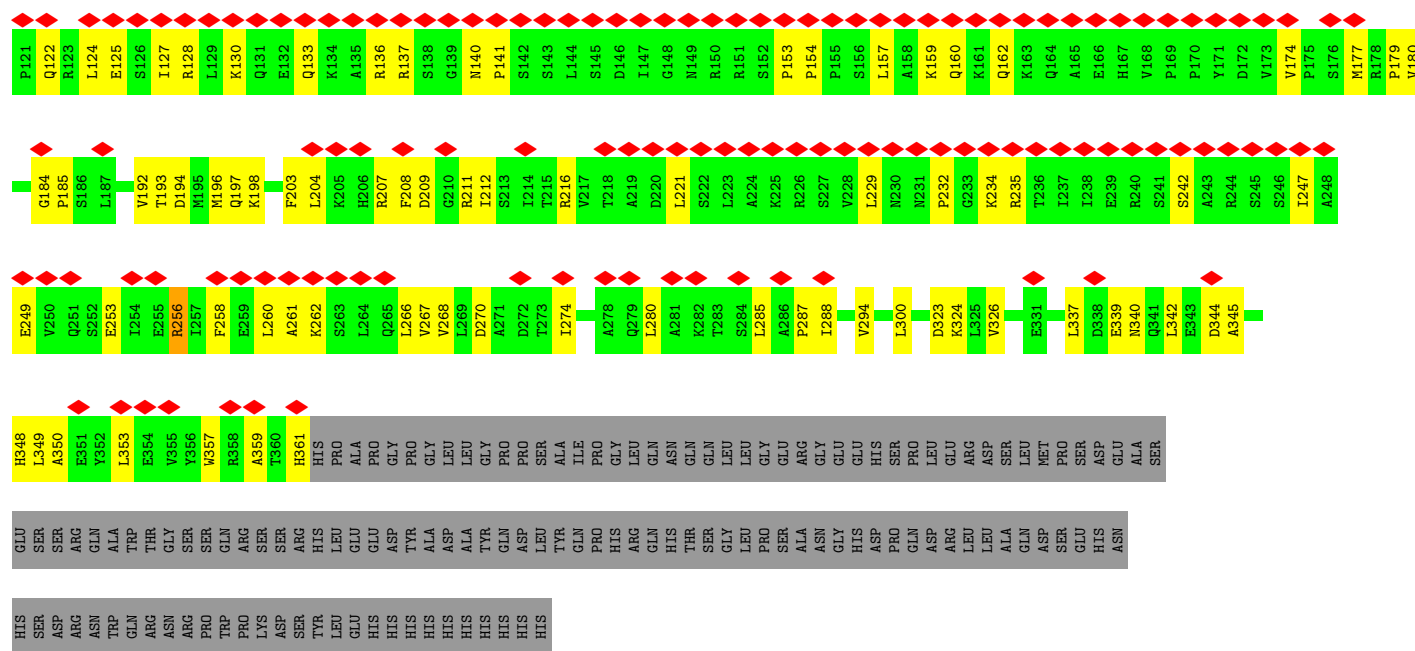
• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1



• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3







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

Chain D: 33% 67%

MAG1  
MAG2  
MAG3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%

MAG1  
MAG2



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1  
NAG2  
NAG3  
NAG4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118997	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.614	Depositor
Minimum map value	-1.578	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.26	Depositor
Map size ( $\text{\AA}$ )	351.328, 351.328, 351.328	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0979, 1.0979, 1.0979	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, 3PE, Y01, PS1, CLR, PT5, CA

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	0/11478	0.47	0/15531
2	B	0.40	0/7858	0.54	0/10658
3	C	0.25	0/2624	0.54	0/3544
All	All	0.32	0/21960	0.50	0/29733

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11202	0	11290	200	0
2	B	7695	0	7485	126	0
3	C	2575	0	2619	66	0
4	D	42	0	37	0	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
6	F	56	0	49	0	0
7	A	38	0	48	3	0
8	A	140	0	230	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	64	0	67	4	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	14	0	13	0	0
11	B	14	0	13	0	0
12	A	105	0	147	24	0
13	A	91	0	139	15	0
All	All	22122	0	22212	399	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 9.

All (399) 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:507:HIS:CE1	12:A:2609:Y01:HAR1	1.86	1.09
1:A:1586:PHE:CD1	8:A:2608:CLR:H21	1.95	1.00
1:A:1658:PHE:HB3	13:A:2614:3PE:H241	1.47	0.97
2:B:41:GLN:HG3	2:B:1009:MET:HB2	1.45	0.95
12:A:2610:Y01:HAA2	13:A:2613:3PE:H3I1	1.47	0.95
1:A:337:TRP:CH2	13:A:2613:3PE:H262	2.07	0.89
1:A:507:HIS:CE1	12:A:2609:Y01:CAR	2.55	0.89
1:A:1656:LEU:HD22	13:A:2614:3PE:O22	1.76	0.86
1:A:657:ILE:CG2	12:A:2606:Y01:HAP2	2.04	0.86
3:C:294:VAL:HG21	3:C:300:LEU:HB2	1.58	0.84
1:A:1835:TRP:CH2	1:A:1846:MET:HB3	2.15	0.81
1:A:507:HIS:NE2	12:A:2609:Y01:HAR1	1.98	0.79
2:B:139:GLU:N	2:B:142:SER:HG	1.81	0.78
1:A:337:TRP:CH2	13:A:2613:3PE:C26	2.67	0.78
1:A:657:ILE:HG21	12:A:2606:Y01:HAP2	1.66	0.77
2:B:537:PRO:HD3	2:B:974:CYS:HB3	1.66	0.77
1:A:507:HIS:CD2	12:A:2609:Y01:HAR1	2.19	0.77
1:A:507:HIS:ND1	12:A:2609:Y01:HAR1	1.98	0.77
1:A:1586:PHE:CD1	8:A:2608:CLR:C2	2.68	0.77
1:A:507:HIS:CG	12:A:2609:Y01:HAR1	2.20	0.76
2:B:653:PHE:HB3	2:B:746:LYS:HZ2	1.50	0.76
1:A:1834:VAL:HB	1:A:1858:MET:HE2	1.66	0.76
2:B:37:VAL:HG21	2:B:1006:GLU:HB3	1.68	0.76
2:B:506:LEU:HD22	2:B:623:LEU:HD21	1.68	0.76
2:B:150:ILE:HG13	2:B:151:GLU:H	1.50	0.76
3:C:184:GLY:HA2	3:C:197:GLN:HE22	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:VAL:HG12	2:B:1047:VAL:HG21	1.68	0.74
1:A:1612:CYS:HG	1:A:1624:TYR:HH	1.33	0.73
1:A:658:MET:HE3	12:A:2606:Y01:HAQ1	1.69	0.73
3:C:203:PHE:HZ	3:C:350:ALA:HB2	1.53	0.73
2:B:823:GLU:OE1	2:B:827:LYS:NZ	2.21	0.73
1:A:731:GLU:O	1:A:735:GLN:NE2	2.23	0.72
2:B:380:LYS:O	2:B:407:LYS:NZ	2.23	0.71
1:A:1612:CYS:SG	1:A:1624:TYR:OH	2.47	0.71
2:B:207:VAL:HG22	2:B:217:TYR:HB3	1.73	0.70
2:B:157:ARG:NH2	2:B:222:PRO:O	2.25	0.70
3:C:212:ILE:HG12	3:C:266:LEU:HB2	1.74	0.69
1:A:249:MET:SD	1:A:1585:LYS:NZ	2.64	0.69
1:A:1520:MET:HG2	1:A:1522:GLU:HG2	1.74	0.69
1:A:658:MET:HE3	12:A:2606:Y01:CAQ	2.24	0.69
3:C:260:LEU:HB3	3:C:267:VAL:HG21	1.74	0.68
3:C:157:LEU:HD23	3:C:162:GLN:HG3	1.76	0.68
2:B:57:LEU:HD21	2:B:715:LEU:HD22	1.76	0.68
1:A:404:LEU:HD13	1:A:474:ARG:HH12	1.59	0.68
1:A:388:GLU:HA	3:C:340:ASN:HD22	1.59	0.67
3:C:180:VAL:HB	3:C:268:VAL:HG12	1.77	0.66
1:A:1526:LEU:HD12	1:A:1907:LYS:HG2	1.79	0.65
1:A:638:GLN:OE1	1:A:680:GLN:NE2	2.30	0.64
1:A:1546:HIS:CD2	1:A:1548:PRO:HD3	2.33	0.64
1:A:658:MET:CE	12:A:2606:Y01:CAQ	2.76	0.64
1:A:1580:ILE:O	1:A:1584:MET:HG3	1.97	0.64
2:B:182:GLU:HA	2:B:185:TRP:CD1	2.33	0.64
1:A:1243:ARG:HH21	1:A:1244:TYR:HE1	1.44	0.63
1:A:337:TRP:CZ2	13:A:2613:3PE:H262	2.34	0.63
1:A:1881:ASP:OD2	1:A:1915:LYS:NZ	2.30	0.63
2:B:496:ASP:OD1	2:B:499:ARG:NH2	2.31	0.63
1:A:1586:PHE:CG	8:A:2608:CLR:H21	2.33	0.63
1:A:1278:TYR:HA	1:A:1281:TYR:HD2	1.64	0.62
1:A:303:ASN:OD1	8:A:2608:CLR:H12	1.99	0.62
1:A:97:TRP:CD1	1:A:99:PRO:HG2	2.35	0.62
1:A:658:MET:CE	12:A:2606:Y01:HAQ2	2.29	0.62
1:A:1835:TRP:CZ3	1:A:1846:MET:HE2	2.35	0.62
2:B:357:ILE:HG22	2:B:383:ARG:HB2	1.82	0.61
2:B:63:LYS:HZ2	2:B:64:TYR:HE1	1.48	0.61
2:B:169:PRO:HG2	2:B:172:ILE:HD13	1.81	0.61
2:B:660:PHE:HB2	2:B:741:THR:HB	1.82	0.61
2:B:166:VAL:HG11	2:B:183:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1583:MET:HE1	8:A:2608:CLR:H231	1.84	0.60
3:C:85:VAL:HG11	3:C:118:ILE:HG22	1.83	0.60
1:A:1701:LEU:HD22	1:A:1800:LEU:HD12	1.81	0.60
2:B:877:GLU:HA	2:B:1030:LEU:HD12	1.84	0.60
3:C:177:MET:H	3:C:261:ALA:HB1	1.67	0.60
1:A:395:TRP:HE1	3:C:196:MET:HA	1.67	0.60
2:B:27:PHE:HZ	2:B:1004:HIS:HB2	1.65	0.59
1:A:657:ILE:HG22	12:A:2606:Y01:HAP2	1.83	0.59
2:B:139:GLU:N	2:B:142:SER:OG	2.35	0.59
2:B:127:ALA:HB2	2:B:165:ALA:HB1	1.84	0.59
1:A:99:PRO:HA	1:A:102:TYR:HB2	1.84	0.59
1:A:403:ILE:HD13	3:C:198:LYS:HE3	1.84	0.59
1:A:1855:LEU:HD21	1:A:1899:LEU:HD21	1.84	0.59
2:B:886:LEU:HD12	2:B:891:VAL:HG11	1.84	0.59
12:A:2610:Y01:CAA	13:A:2613:3PE:H3I1	2.28	0.59
3:C:179:PRO:HG2	3:C:287:PRO:HB3	1.84	0.59
1:A:1333:SER:O	1:A:1336:LYS:HG2	2.03	0.59
1:A:1731:GLN:HG3	1:A:1759:ASN:HB3	1.84	0.59
1:A:309:LEU:HD13	1:A:694:ILE:HD11	1.83	0.58
1:A:382:GLN:O	1:A:386:GLU:HG2	2.03	0.58
1:A:658:MET:HE2	12:A:2606:Y01:HAQ2	1.84	0.58
3:C:323:ASP:OD1	3:C:324:LYS:N	2.36	0.58
1:A:392:TYR:O	1:A:396:ILE:HG12	2.03	0.58
2:B:889:ILE:HG13	2:B:891:VAL:HG23	1.86	0.58
1:A:1344:LEU:HD13	1:A:1347:LEU:HD12	1.84	0.58
2:B:508:PRO:HG2	2:B:764:TYR:HE2	1.70	0.57
1:A:1639:GLY:HA3	1:A:1662:PHE:HD2	1.70	0.57
2:B:273:ARG:HD2	2:B:323:ASN:HA	1.87	0.57
1:A:1378:ASN:OD1	1:A:1379:ILE:N	2.38	0.56
2:B:29:SER:HB3	2:B:32:THR:HG23	1.87	0.56
3:C:185:PRO:HD2	3:C:193:THR:HG22	1.86	0.56
1:A:1923:ARG:NH2	1:A:1942:VAL:O	2.39	0.56
1:A:220:MET:O	1:A:224:ILE:HG12	2.06	0.56
1:A:265:GLN:HG3	1:A:285:THR:HG21	1.88	0.56
1:A:387:ARG:NH1	1:A:729:GLU:OE2	2.39	0.56
1:A:1586:PHE:CG	8:A:2608:CLR:C2	2.89	0.56
1:A:1834:VAL:HB	1:A:1858:MET:CE	2.35	0.56
1:A:337:TRP:CH2	13:A:2613:3PE:H261	2.40	0.56
1:A:1497:PHE:HB2	1:A:1498:PRO:HD3	1.88	0.56
1:A:97:TRP:HD1	1:A:99:PRO:HG2	1.71	0.56
1:A:1643:ASP:OD2	1:A:1663:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:TRP:CZ3	1:A:1846:MET:CE	2.89	0.55
2:B:714:GLU:OE2	2:B:718:ASN:ND2	2.40	0.55
1:A:1499:PHE:O	1:A:1503:ASN:ND2	2.35	0.55
3:C:337:LEU:HD22	3:C:345:ALA:HB1	1.88	0.55
2:B:660:PHE:HD1	2:B:676:ASN:HD22	1.53	0.55
1:A:587:LEU:HD13	9:A:2603:PT5:H26	1.87	0.55
8:A:2602:CLR:H162	8:A:2602:CLR:H272	1.89	0.54
2:B:295:ASN:OD1	2:B:296:SER:N	2.33	0.54
3:C:184:GLY:HA2	3:C:197:GLN:NE2	2.21	0.54
3:C:280:LEU:HD11	3:C:285:LEU:HD12	1.89	0.54
1:A:1326:ALA:HB2	1:A:1344:LEU:HB3	1.90	0.54
2:B:160:SER:HB3	2:B:220:ALA:HB3	1.90	0.54
2:B:595:GLN:HB3	2:B:762:SER:HB3	1.89	0.54
2:B:508:PRO:HG2	2:B:764:TYR:CE2	2.43	0.54
2:B:653:PHE:HB3	2:B:746:LYS:NZ	2.22	0.54
1:A:1235:LEU:O	1:A:1239:ILE:HG12	2.08	0.53
1:A:1262:ALA:O	1:A:1272:ARG:NE	2.41	0.53
1:A:1410:LYS:HD2	1:A:1415:ASP:HB3	1.89	0.53
1:A:1862:LEU:HD11	1:A:1899:LEU:HB3	1.91	0.53
2:B:775:PHE:HE1	2:B:1011:THR:HB	1.73	0.53
1:A:339:TYR:HB2	13:A:2614:3PE:H341	1.91	0.53
1:A:1729:GLU:OE2	1:A:1768:LYS:NZ	2.40	0.53
3:C:194:ASP:HB3	3:C:198:LYS:NZ	2.23	0.53
1:A:1646:VAL:HG21	1:A:1655:ASN:HD22	1.74	0.53
1:A:550:PHE:HZ	9:A:2603:PT5:H17	1.74	0.53
1:A:151:LYS:HE3	1:A:164:TYR:HE1	1.74	0.53
2:B:150:ILE:HG13	2:B:151:GLU:N	2.20	0.53
1:A:1304:GLN:HA	1:A:1309:ARG:HH21	1.74	0.52
2:B:309:GLN:HE21	2:B:311:ASN:HD21	1.58	0.52
2:B:777:ALA:HA	2:B:860:LEU:HD21	1.92	0.52
1:A:1527:GLU:O	1:A:1531:ARG:NH1	2.43	0.52
1:A:1657:SER:HB3	1:A:1660:ARG:HE	1.74	0.52
1:A:747:GLU:HA	3:C:110:LYS:HE2	1.92	0.52
1:A:1891:HIS:CE1	1:A:1940:LEU:HD21	2.45	0.52
2:B:397:GLY:H	2:B:398:PRO:HD2	1.75	0.52
1:A:550:PHE:CZ	9:A:2603:PT5:H17	2.46	0.52
1:A:1769:PRO:HD3	1:A:1779:ARG:HH21	1.75	0.51
2:B:497:ILE:HG22	2:B:523:LEU:HD11	1.93	0.51
3:C:258:PHE:O	3:C:262:LYS:HG3	2.09	0.51
2:B:733:PHE:CZ	2:B:813:GLY:HA3	2.44	0.51
1:A:1835:TRP:CD1	1:A:1892:PHE:CD1	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:PHE:HD2	2:B:883:MET:SD	2.33	0.51
2:B:1028:THR:O	2:B:1029:ARG:C	2.49	0.51
1:A:157:PHE:HB2	1:A:164:TYR:H	1.74	0.51
1:A:341:ILE:HD13	13:A:2613:3PE:H372	1.91	0.51
13:A:2614:3PE:H2	13:A:2614:3PE:H111	1.92	0.51
3:C:204:LEU:HD11	3:C:349:LEU:HD23	1.93	0.51
3:C:344:ASP:OD1	3:C:345:ALA:N	2.43	0.51
1:A:1256:SER:HB3	1:A:1351:ARG:HD3	1.92	0.50
1:A:1272:ARG:CG	8:A:2611:CLR:H191	2.42	0.50
1:A:1802:LEU:HD22	7:A:2601:PS1:H23	1.92	0.50
3:C:179:PRO:O	3:C:288:ILE:N	2.35	0.50
2:B:713:ASN:O	2:B:717:GLN:HG2	2.11	0.50
2:B:736:THR:HG23	2:B:810:ALA:HB2	1.93	0.50
1:A:1605:THR:HG21	1:A:1644:ILE:CD1	2.41	0.50
2:B:615:THR:HG22	2:B:617:TYR:H	1.77	0.50
1:A:1369:VAL:HG22	1:A:1803:ASN:HD22	1.76	0.50
3:C:208:PHE:CE2	3:C:353:LEU:HD11	2.46	0.50
1:A:1496:VAL:O	1:A:1500:PHE:HB3	2.12	0.49
2:B:409:TYR:HD2	2:B:411:TYR:CZ	2.31	0.49
2:B:731:ALA:HB3	2:B:815:LYS:HG3	1.94	0.49
1:A:1369:VAL:HG22	1:A:1803:ASN:ND2	2.28	0.49
1:A:1851:MET:O	1:A:1854:MET:HB3	2.13	0.49
2:B:301:VAL:HG12	2:B:321:ALA:HB1	1.95	0.49
1:A:741:LYS:HG3	3:C:348:HIS:CD2	2.47	0.49
1:A:1661:LEU:HD11	13:A:2614:3PE:H371	1.95	0.49
1:A:388:GLU:HA	3:C:340:ASN:ND2	2.26	0.49
2:B:204:LEU:HD13	2:B:456:LEU:HD13	1.94	0.49
3:C:46:SER:O	3:C:50:GLN:HG2	2.13	0.49
2:B:770:ASN:HD22	2:B:774:VAL:HG22	1.78	0.48
1:A:1564:SER:OG	1:A:1566:PRO:HD2	2.14	0.48
8:A:2611:CLR:H162	8:A:2611:CLR:H221	1.37	0.48
2:B:421:ILE:O	2:B:425:GLU:HG2	2.14	0.48
3:C:192:VAL:O	3:C:196:MET:HG2	2.13	0.48
2:B:877:GLU:HG3	2:B:1030:LEU:HG	1.96	0.48
2:B:601:ASP:OD1	2:B:602:LYS:N	2.46	0.48
3:C:203:PHE:CD2	3:C:204:LEU:HD12	2.49	0.48
1:A:1502:VAL:HG21	8:A:2602:CLR:H151	1.96	0.48
1:A:727:GLN:O	1:A:730:GLU:HG3	2.13	0.48
1:A:472:GLU:O	1:A:476:ARG:HG3	2.14	0.47
13:A:2613:3PE:H221	13:A:2613:3PE:H252	1.47	0.47
2:B:999:CYS:HB3	2:B:1024:CYS:HB3	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1567:PHE:O	1:A:1571:ILE:HG12	2.14	0.47
1:A:1901:ARG:HG3	1:A:1906:ILE:HB	1.97	0.47
3:C:357:TRP:O	3:C:361:HIS:ND1	2.46	0.47
3:C:221:LEU:HB3	3:C:274:ILE:HD11	1.96	0.47
1:A:283:ASN:OD1	1:A:283:ASN:N	2.47	0.47
1:A:1784:GLU:HB2	8:A:2612:CLR:H12	1.95	0.47
7:A:2601:PS1:H7	8:A:2602:CLR:C19	2.44	0.47
2:B:79:VAL:HG22	2:B:610:THR:HG22	1.97	0.47
3:C:242:SER:HB3	3:C:247:ILE:HD11	1.95	0.47
1:A:501:LEU:O	1:A:505:ILE:HG12	2.14	0.47
1:A:1722:ASP:OD1	1:A:1723:GLU:N	2.45	0.47
2:B:843:ARG:NH2	2:B:863:ASN:O	2.44	0.47
1:A:1882:LEU:HD12	1:A:1883:PRO:HD2	1.96	0.47
2:B:719:TYR:HD2	2:B:720:TRP:HD1	1.61	0.47
2:B:1054:LYS:HB3	2:B:1054:LYS:HE2	1.32	0.47
3:C:159:LYS:HG2	3:C:160:GLN:H	1.80	0.47
2:B:47:LEU:HD11	2:B:728:GLY:HA3	1.97	0.46
1:A:553:PHE:O	1:A:557:VAL:HG23	2.16	0.46
3:C:95:ILE:HD11	3:C:118:ILE:HD11	1.97	0.46
1:A:215:VAL:O	1:A:219:ILE:HG13	2.15	0.46
1:A:264:ILE:HG21	1:A:269:PRO:HG3	1.98	0.46
1:A:1905:ASP:HA	1:A:1908:ILE:HD12	1.96	0.46
13:A:2614:3PE:H252	13:A:2614:3PE:H351	1.98	0.46
2:B:975:ILE:HD12	2:B:1040:GLY:H	1.80	0.46
1:A:465:SER:OG	1:A:466:THR:N	2.48	0.46
1:A:1605:THR:HG21	1:A:1644:ILE:HD11	1.97	0.46
2:B:797:ALA:HA	2:B:811:VAL:HG22	1.96	0.46
3:C:209:ASP:O	3:C:211:ARG:NH1	2.48	0.46
3:C:229:LEU:HB3	3:C:232:PRO:HG3	1.96	0.46
2:B:829:SER:HB2	2:B:840:ASP:OD2	2.16	0.46
2:B:1003:PHE:HB3	2:B:1018:VAL:HG23	1.98	0.46
3:C:323:ASP:HA	3:C:326:VAL:HG22	1.96	0.46
12:A:2606:Y01:HAM1	12:A:2606:Y01:HBC	1.39	0.46
2:B:532:ILE:HD13	2:B:901:GLN:HG3	1.96	0.46
2:B:648:LEU:H	2:B:648:LEU:HD23	1.80	0.46
2:B:682:ASN:O	2:B:686:PHE:CD2	2.69	0.46
3:C:77:GLU:HB2	3:C:103:TRP:HZ2	1.81	0.46
1:A:564:GLU:OE1	1:A:578:ILE:HG22	2.16	0.46
1:A:508:TYR:OH	1:A:1475:ASN:ND2	2.45	0.46
1:A:1395:VAL:O	1:A:1399:LYS:HB2	2.15	0.46
1:A:1534:ILE:O	1:A:1538:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:HG11	1:A:216:LEU:HD12	1.98	0.46
1:A:480:ARG:HG2	1:A:484:LYS:NZ	2.31	0.46
1:A:1680:LEU:HD13	1:A:1815:TYR:HE2	1.81	0.46
2:B:743:VAL:HG22	2:B:745:PRO:HD2	1.97	0.46
1:A:1272:ARG:NH1	12:A:2610:Y01:HAM2	2.31	0.45
2:B:640:THR:HG22	2:B:643:ARG:HH22	1.80	0.45
2:B:764:TYR:O	2:B:768:LEU:HD23	2.17	0.45
3:C:125:GLU:HG3	3:C:128:ARG:HH21	1.80	0.45
1:A:653:PHE:HB3	1:A:654:PRO:HD3	1.98	0.45
2:B:147:PRO:HG2	2:B:149:PHE:CZ	2.51	0.45
3:C:203:PHE:CE1	3:C:207:ARG:HG3	2.51	0.45
1:A:519:TYR:CZ	1:A:523:PHE:HE2	2.35	0.45
1:A:1263:GLU:HG2	1:A:1276:LEU:HD13	1.99	0.45
1:A:1488:ILE:HD11	12:A:2606:Y01:HAD2	1.98	0.45
2:B:778:PRO:HG3	2:B:787:ALA:HB2	1.98	0.45
1:A:1390:PHE:CE1	8:A:2607:CLR:H242	2.51	0.45
2:B:182:GLU:HG2	2:B:185:TRP:HE1	1.81	0.45
3:C:216:ARG:HA	3:C:270:ASP:HB2	1.97	0.45
2:B:301:VAL:HG13	2:B:325:ILE:HD11	1.97	0.45
1:A:1625:PHE:O	1:A:1631:ILE:HD11	2.17	0.45
1:A:395:TRP:HD1	1:A:396:ILE:HD13	1.81	0.45
2:B:744:TYR:HB3	2:B:745:PRO:HD3	1.99	0.45
3:C:130:LYS:O	3:C:133:GLN:HG3	2.17	0.45
1:A:1864:LEU:HD21	1:A:1876:ARG:HD3	1.98	0.45
2:B:29:SER:O	2:B:33:ILE:HG12	2.17	0.45
2:B:1030:LEU:H	2:B:1030:LEU:HD22	1.81	0.45
2:B:28:PRO:HB2	2:B:33:ILE:HG23	2.00	0.44
2:B:147:PRO:HB3	2:B:163:HIS:CE1	2.52	0.44
2:B:193:PHE:HB3	2:B:218:TYR:CG	2.52	0.44
1:A:483:VAL:HG11	1:A:540:LEU:HD11	1.99	0.44
1:A:1301:VAL:HG13	1:A:1301:VAL:O	2.17	0.44
1:A:164:TYR:HE2	1:A:174:PHE:HB2	1.83	0.44
2:B:516:ASP:OD1	2:B:520:TYR:N	2.50	0.44
2:B:637:GLU:O	2:B:641:GLN:HG2	2.16	0.44
3:C:80:VAL:HB	3:C:117:PHE:CE2	2.52	0.44
3:C:157:LEU:HA	3:C:162:GLN:HG3	1.98	0.44
1:A:1417:ARG:NH2	2:B:173:TYR:OH	2.51	0.44
1:A:1718:ILE:HG12	1:A:1739:ARG:NH2	2.32	0.44
2:B:847:VAL:HG13	2:B:848:MET:N	2.33	0.44
2:B:99:ARG:HD2	2:B:196:ASN:OD1	2.17	0.44
1:A:337:TRP:CZ2	13:A:2613:3PE:C26	2.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:VAL:O	1:A:1396:GLN:HG2	2.17	0.44
1:A:1500:PHE:CZ	1:A:1504:ILE:HD11	2.53	0.44
1:A:1558:MET:O	1:A:1562:VAL:HG23	2.17	0.44
2:B:840:ASP:OD1	2:B:841:CYS:N	2.45	0.44
3:C:234:LYS:HG3	3:C:235:ARG:HG2	2.00	0.44
2:B:1021:LYS:H	2:B:1021:LYS:HD2	1.82	0.44
2:B:1021:LYS:HE2	2:B:1021:LYS:HB3	1.86	0.44
2:B:89:LEU:HD22	2:B:500:LEU:HD11	1.99	0.44
2:B:103:GLU:HG2	2:B:192:VAL:HG21	2.00	0.44
2:B:108:GLN:HG2	2:B:485:LEU:HD11	1.98	0.44
2:B:650:PRO:HA	2:B:653:PHE:CZ	2.53	0.44
1:A:1340:THR:O	1:A:1344:LEU:HD23	2.18	0.44
1:A:1640:SER:OG	1:A:1666:ARG:NH2	2.51	0.44
2:B:124:TYR:CE1	2:B:183:LEU:HD13	2.52	0.44
1:A:1901:ARG:HA	1:A:1906:ILE:HD12	2.00	0.43
2:B:719:TYR:HD2	2:B:720:TRP:CD1	2.35	0.43
1:A:254:THR:HG22	1:A:272:CYS:SG	2.58	0.43
1:A:589:ILE:O	1:A:592:VAL:HG22	2.18	0.43
1:A:1627:ASP:O	1:A:1631:ILE:HD12	2.18	0.43
9:A:2603:PT5:H45	9:A:2603:PT5:H39	1.78	0.43
2:B:442:LYS:NZ	2:B:465:PRO:O	2.45	0.43
1:A:232:LEU:HD21	1:A:1677:ILE:HG23	2.00	0.43
1:A:389:LEU:O	1:A:393:MET:HG2	2.19	0.43
1:A:1339:ASN:OD1	1:A:1340:THR:N	2.52	0.43
2:B:366:GLU:N	2:B:366:GLU:OE1	2.51	0.43
2:B:1028:THR:O	2:B:1030:LEU:HD13	2.18	0.43
3:C:253:GLU:HA	3:C:256:ARG:HH21	1.83	0.43
1:A:1643:ASP:HB2	1:A:1659:LEU:HB3	2.00	0.43
8:A:2602:CLR:H192	8:A:2602:CLR:H22	1.55	0.43
2:B:193:PHE:CG	2:B:218:TYR:HB2	2.54	0.43
1:A:192:ARG:H	1:A:192:ARG:HG3	1.60	0.43
1:A:1329:PHE:C	1:A:1331:GLY:H	2.22	0.43
2:B:896:LYS:HB3	2:B:896:LYS:HE3	1.33	0.43
3:C:249:GLU:O	3:C:253:GLU:HG2	2.18	0.43
1:A:331:SER:O	1:A:331:SER:OG	2.31	0.43
2:B:682:ASN:O	2:B:686:PHE:HD2	2.01	0.43
3:C:109:VAL:O	3:C:359:ALA:HB1	2.19	0.43
1:A:550:PHE:HB3	1:A:588:ARG:NH2	2.33	0.43
2:B:54:VAL:HG23	2:B:55:ASN:H	1.83	0.43
2:B:824:ASN:HA	2:B:827:LYS:HZ2	1.83	0.43
3:C:203:PHE:CZ	3:C:350:ALA:HB2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HA	1:A:141:ILE:HG22	2.00	0.43
1:A:1291:MET:SD	1:A:1320:VAL:HG11	2.59	0.43
1:A:395:TRP:CZ3	3:C:342:LEU:HA	2.53	0.43
8:A:2602:CLR:H182	8:A:2602:CLR:H8	1.60	0.43
1:A:742:ALA:HA	1:A:745:VAL:HG12	2.00	0.43
1:A:1639:GLY:HA3	1:A:1662:PHE:CD2	2.52	0.43
1:A:507:HIS:CE1	12:A:2609:Y01:HAR2	2.46	0.42
1:A:507:HIS:ND1	12:A:2609:Y01:CAR	2.76	0.42
1:A:1378:ASN:OD1	1:A:1379:ILE:HG12	2.18	0.42
7:A:2601:PS1:H7	8:A:2602:CLR:H192	2.01	0.42
2:B:726:ILE:HB	2:B:729:VAL:HB	2.01	0.42
3:C:140:ASN:OD1	3:C:141:PRO:HD3	2.19	0.42
1:A:135:ASP:O	1:A:138:PRO:HD2	2.19	0.42
1:A:1703:PHE:O	1:A:1707:ILE:HG12	2.19	0.42
2:B:662:ALA:HA	2:B:663:PRO:HD3	1.91	0.42
2:B:882:LEU:O	2:B:886:LEU:HD23	2.19	0.42
1:A:1718:ILE:HG22	1:A:1732:ILE:HG22	2.01	0.42
1:A:1272:ARG:HD2	8:A:2611:CLR:H182	2.01	0.42
2:B:218:TYR:HB3	2:B:219:PRO:HD3	2.01	0.42
2:B:363:ASP:OD1	2:B:364:GLY:N	2.53	0.42
1:A:87:VAL:HA	1:A:156:GLY:HA2	2.01	0.42
1:A:726:GLU:HA	1:A:729:GLU:HG3	2.02	0.42
2:B:642:ALA:O	2:B:646:GLU:HG2	2.19	0.42
1:A:122:PRO:HG3	1:A:640:ASN:ND2	2.35	0.42
1:A:627:PHE:CD1	1:A:696:LEU:HD13	2.55	0.42
2:B:661:ILE:H	2:B:676:ASN:HD21	1.67	0.42
1:A:629:LEU:O	1:A:633:GLN:HG2	2.20	0.42
1:A:1377:PHE:O	1:A:1381:ILE:HG12	2.20	0.42
1:A:1725:SER:O	1:A:1726:ASP:C	2.58	0.42
2:B:713:ASN:HA	2:B:716:VAL:HG12	2.02	0.42
1:A:206:VAL:HG11	1:A:216:LEU:CD1	2.49	0.42
1:A:620:LEU:HD23	12:A:2606:Y01:CAB	2.49	0.42
1:A:1292:VAL:O	1:A:1296:ILE:HG12	2.19	0.42
1:A:1690:ALA:O	1:A:1692:PRO:HD3	2.20	0.42
1:A:1726:ASP:HB3	1:A:1730:PHE:HD2	1.85	0.42
2:B:779:TYR:HB3	2:B:782:LYS:HG3	2.00	0.42
2:B:514:ALA:HB3	2:B:522:LEU:HB3	2.02	0.41
3:C:58:LYS:HE2	3:C:97:GLU:HB3	2.02	0.41
3:C:136:ARG:O	3:C:137:ARG:NH1	2.45	0.41
3:C:153:PRO:HA	3:C:154:PRO:HD3	1.92	0.41
1:A:1401:LYS:HB3	1:A:1471:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:2610:Y01:HAP1	12:A:2610:Y01:HAO2	1.68	0.41
1:A:492:VAL:O	1:A:496:VAL:HG23	2.20	0.41
2:B:33:ILE:HD12	2:B:1004:HIS:ND1	2.36	0.41
2:B:735:VAL:HG21	2:B:763:PHE:CZ	2.55	0.41
1:A:1641:ILE:O	1:A:1645:LEU:HG	2.20	0.41
2:B:344:LEU:HD23	2:B:344:LEU:HA	1.92	0.41
1:A:376:PHE:CZ	1:A:721:GLU:HB3	2.55	0.41
2:B:682:ASN:O	2:B:685:GLU:HG3	2.21	0.41
1:A:1519:LYS:HE2	1:A:1519:LYS:HB2	1.86	0.41
1:A:1633:ASP:OD1	1:A:1669:LYS:HD3	2.20	0.41
1:A:1634:PHE:CE2	1:A:1638:LEU:HD11	2.55	0.41
3:C:65:ARG:HD2	3:C:174:VAL:HG11	2.02	0.41
3:C:85:VAL:HG23	3:C:108:LEU:HD11	2.03	0.41
2:B:54:VAL:HG23	2:B:55:ASN:N	2.36	0.41
2:B:841:CYS:HB3	2:B:863:ASN:HD22	1.85	0.41
1:A:470:LYS:HA	1:A:470:LYS:HD3	1.86	0.41
1:A:1272:ARG:HG3	8:A:2611:CLR:H191	2.03	0.41
1:A:281:CYS:HB3	1:A:285:THR:OG1	2.21	0.41
1:A:661:PHE:O	1:A:665:THR:HG23	2.20	0.41
1:A:1284:THR:O	1:A:1288:THR:HG23	2.20	0.41
1:A:1291:MET:O	1:A:1295:MET:HG2	2.20	0.41
1:A:1378:ASN:O	1:A:1382:VAL:HG23	2.20	0.41
12:A:2610:Y01:HAA3	12:A:2610:Y01:HAJ2	1.75	0.41
2:B:746:LYS:HD3	2:B:746:LYS:HA	1.76	0.41
3:C:193:THR:O	3:C:197:GLN:OE1	2.38	0.41
1:A:392:TYR:OH	3:C:294:VAL:HA	2.20	0.41
2:B:892:TYR:HE1	2:B:983:PHE:CE1	2.39	0.41
3:C:70:TYR:CZ	3:C:127:ILE:HG12	2.56	0.41
1:A:1272:ARG:HD3	8:A:2611:CLR:C19	2.51	0.40
1:A:299:THR:HG21	1:A:323:LEU:HD11	2.02	0.40
2:B:147:PRO:HB3	2:B:163:HIS:NE2	2.36	0.40
1:A:555:CYS:O	1:A:559:ILE:HG12	2.22	0.40
1:A:622:LEU:HD23	1:A:622:LEU:HA	1.88	0.40
8:A:2602:CLR:H193	8:A:2602:CLR:H111	1.48	0.40
2:B:868:THR:O	2:B:871:ILE:HG12	2.21	0.40
3:C:102:ASP:OD2	3:C:103:TRP:NE1	2.55	0.40
3:C:119:PRO:HB2	3:C:124:LEU:HG	2.02	0.40
3:C:159:LYS:HG2	3:C:160:GLN:N	2.37	0.40
1:A:725:ASP:O	1:A:728:GLU:HG2	2.22	0.40
2:B:139:GLU:N	2:B:140:PRO:HD2	2.36	0.40
3:C:94:HIS:HB2	3:C:107:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:TRP:CH2	1:A:1846:MET:CB	2.96	0.40
2:B:1027:ASP:HB3	2:B:1029:ARG:HH21	1.86	0.40
3:C:102:ASP:HA	3:C:122:GLN:HE21	1.86	0.40
3:C:339:GLU:OE1	3:C:339:GLU:N	2.54	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	1368/2549 (54%)	1323 (97%)	45 (3%)	0	100	100
2	B	954/1115 (86%)	902 (94%)	52 (6%)	0	100	100
3	C	322/496 (65%)	312 (97%)	10 (3%)	0	100	100
All	All	2644/4160 (64%)	2537 (96%)	107 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1214/2154 (56%)	1206 (99%)	8 (1%)	81	90
2	B	854/983 (87%)	819 (96%)	35 (4%)	26	51
3	C	287/438 (66%)	286 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2355/3575 (66%)	2311 (98%)	44 (2%)	54 73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	192	ARG
1	A	283	ASN
1	A	608	ASN
1	A	699[A]	PHE
1	A	699[B]	PHE
1	A	1334	LYS
1	A	1611	GLU
2	B	713	ASN
2	B	895	ASN
2	B	896	LYS
2	B	897	SER
2	B	902	SER
2	B	903	VAL
2	B	974	CYS
2	B	976	THR
2	B	979	THR
2	B	985	ASN
2	B	987	SER
2	B	989	SER
2	B	991	SER
2	B	993	VAL
2	B	994	LEU
2	B	1009	MET
2	B	1012	ASN
2	B	1016	ILE
2	B	1021	LYS
2	B	1029	ARG
2	B	1030	LEU
2	B	1033	GLN
2	B	1038	SER
2	B	1039	ASP
2	B	1047	VAL
2	B	1053	ARG
2	B	1054	LYS
2	B	1058	VAL
2	B	1063	ASN

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Mol	Chain	Res	Type
2	B	1064	VAL
2	B	1068	TYR
2	B	1069	THR
2	B	1071	CYS
2	B	1074	VAL
2	B	1075	SER
3	C	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	735	GLN
1	A	1803	ASN
2	B	309	GLN
2	B	676	ASN
2	B	1012	ASN
2	B	1042	ASN
3	C	122	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 ⓘ

13 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
4	NAG	D	1	2,4	14,14,15	0.54	0	17,19,21	1.93	5 (29%)
4	NAG	D	2	4	14,14,15	0.38	0	17,19,21	1.54	3 (17%)
4	NAG	D	3	4	14,14,15	0.32	0	17,19,21	0.87	0
5	NAG	E	1	2,5	14,14,15	0.62	0	17,19,21	1.30	2 (11%)
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	0.58	0
6	NAG	F	1	6	14,14,15	0.76	0	17,19,21	1.52	2 (11%)
6	NAG	F	2	6	14,14,15	0.52	0	17,19,21	1.55	3 (17%)
6	NAG	F	3	6	14,14,15	0.42	0	17,19,21	1.96	4 (23%)
6	NAG	F	4	6	14,14,15	0.42	0	17,19,21	1.22	2 (11%)
5	NAG	G	1	2,5	14,14,15	0.66	0	17,19,21	1.31	2 (11%)
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
5	NAG	H	1	2,5	14,14,15	0.49	0	17,19,21	2.04	5 (29%)
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.39	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
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	NAG	D	3	4	-	5/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	5/6/23/26	0/1/1/1
6	NAG	F	4	6	-	6/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	NAG	C1-O5-C5	4.68	118.54	112.19
5	H	1	NAG	C4-C3-C2	-4.40	104.57	111.02
6	F	3	NAG	C3-C4-C5	4.20	117.73	110.24
4	D	1	NAG	C1-O5-C5	4.16	117.83	112.19
6	F	1	NAG	O5-C1-C2	-4.00	104.98	111.29
4	D	2	NAG	C2-N2-C7	3.90	128.46	122.90
6	F	3	NAG	C4-C3-C2	3.65	116.36	111.02
5	H	1	NAG	C2-N2-C7	3.59	128.01	122.90
5	H	1	NAG	C1-O5-C5	3.58	117.04	112.19
6	F	2	NAG	O5-C1-C2	-3.54	105.69	111.29
5	G	1	NAG	C1-O5-C5	-3.49	107.47	112.19
5	E	1	NAG	C4-C3-C2	3.27	115.81	111.02
4	D	2	NAG	C1-C2-N2	3.24	116.03	110.49
6	F	2	NAG	O3-C3-C2	-3.19	102.87	109.47
4	D	1	NAG	C4-C3-C2	3.12	115.59	111.02
6	F	2	NAG	C2-N2-C7	-3.01	118.62	122.90
5	G	2	NAG	O5-C1-C2	-2.96	106.62	111.29
4	D	1	NAG	C3-C4-C5	2.90	115.40	110.24
4	D	1	NAG	O5-C1-C2	-2.88	106.73	111.29
6	F	4	NAG	O5-C1-C2	2.77	115.66	111.29
4	D	1	NAG	O5-C5-C6	-2.69	102.98	107.20
5	H	1	NAG	C1-C2-N2	2.61	114.95	110.49
6	F	4	NAG	C4-C3-C2	2.49	114.66	111.02
6	F	1	NAG	C4-C3-C2	2.47	114.64	111.02
5	H	1	NAG	O4-C4-C5	2.41	115.27	109.30
5	G	1	NAG	C4-C3-C2	2.36	114.48	111.02
4	D	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	E	1	NAG	O5-C5-C6	-2.23	103.71	107.20
6	F	3	NAG	O5-C5-C4	2.14	116.03	110.83

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	NAG	C8-C7-N2-C2
4	D	3	NAG	O7-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2

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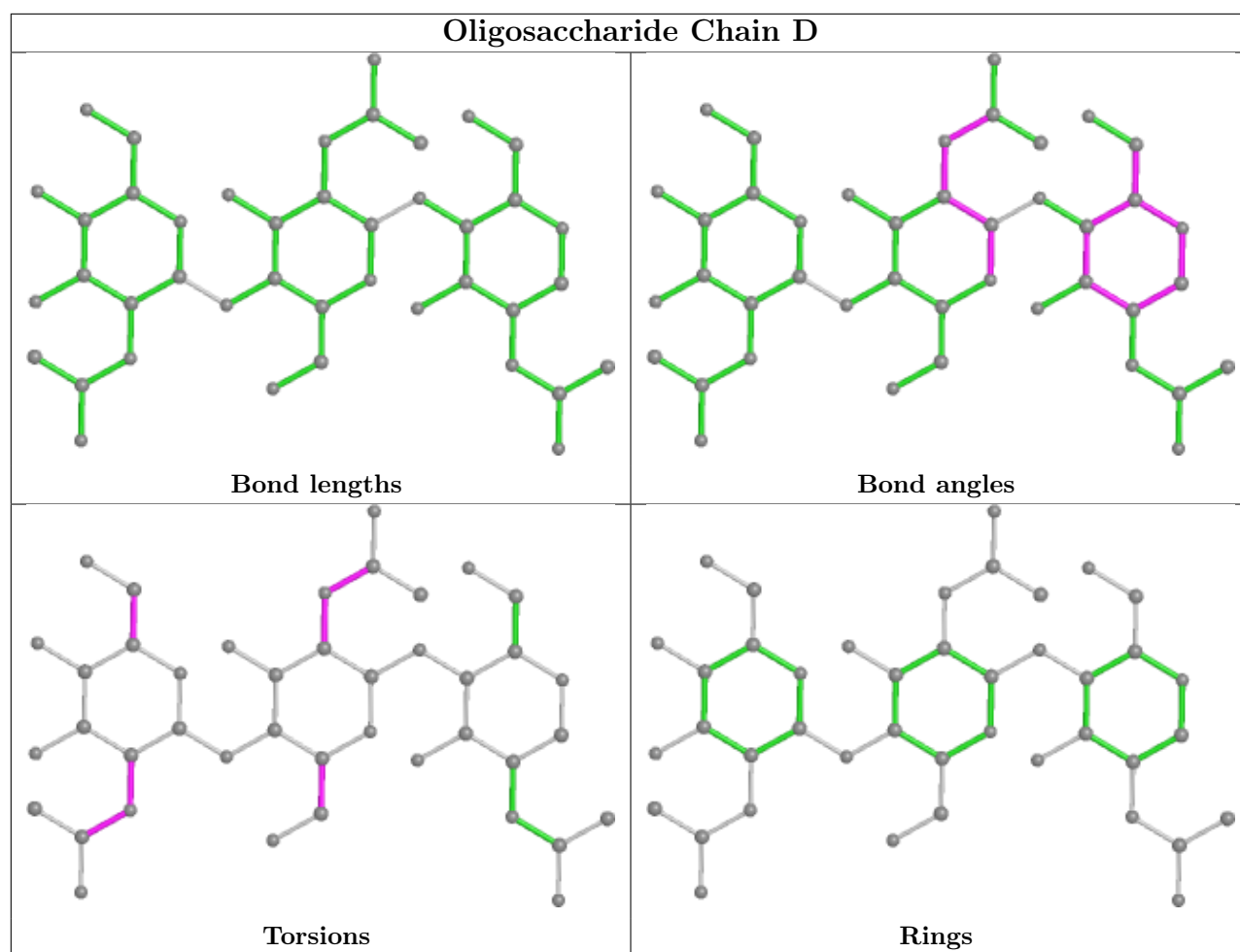
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O7-C7-N2-C2
6	F	3	NAG	C3-C2-N2-C7
6	F	3	NAG	C8-C7-N2-C2
6	F	3	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
6	F	3	NAG	C4-C5-C6-O6
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
4	D	3	NAG	C1-C2-N2-C7
5	G	1	NAG	C4-C5-C6-O6
6	F	4	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C1-C2-N2-C7
4	D	3	NAG	C4-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
6	F	4	NAG	C4-C5-C6-O6
5	G	1	NAG	O7-C7-N2-C2
4	D	3	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	F	4	NAG	C1-C2-N2-C7
6	F	4	NAG	C3-C2-N2-C7

There are no ring outliers.

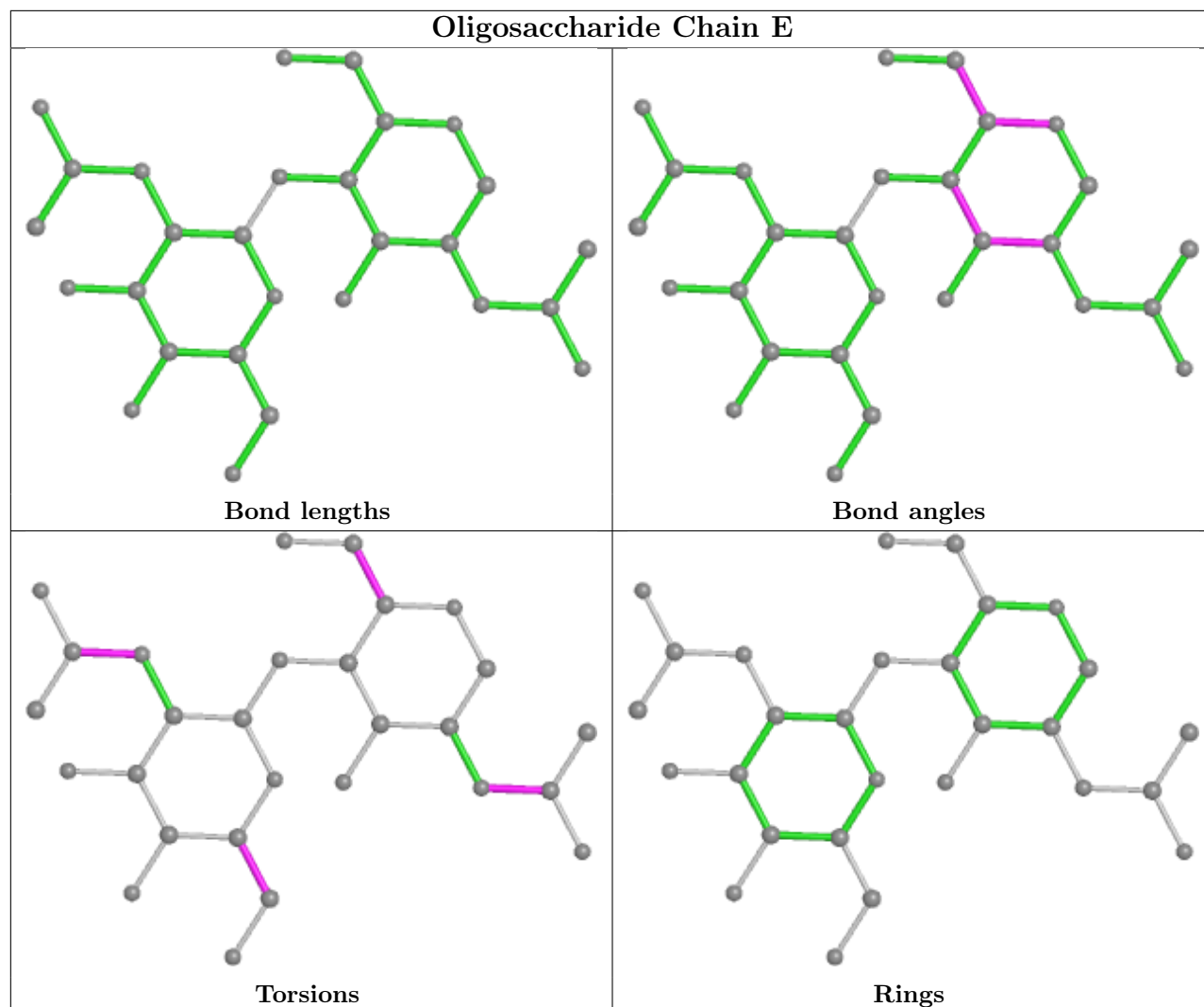
No monomer is involved in short contacts.

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

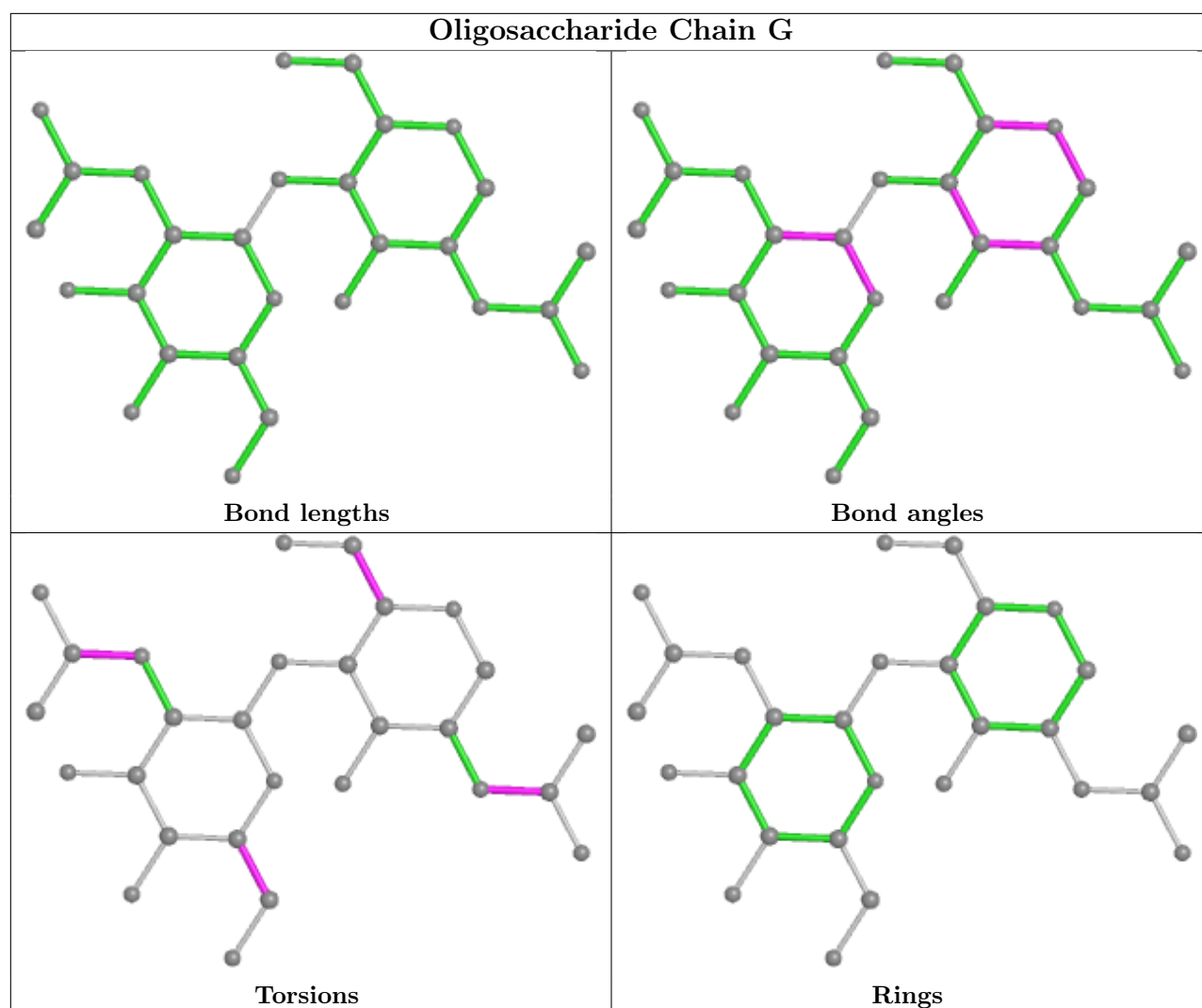




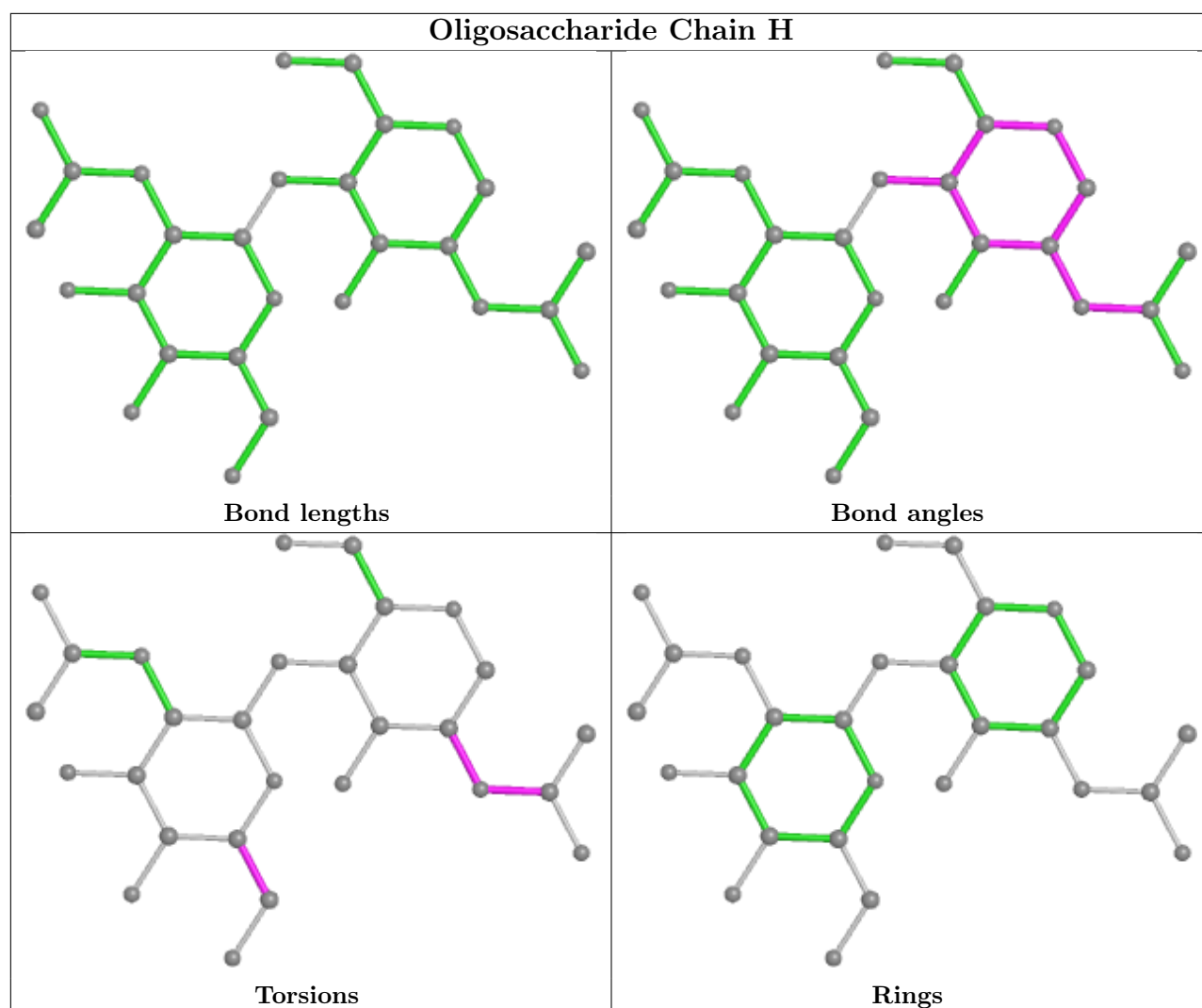




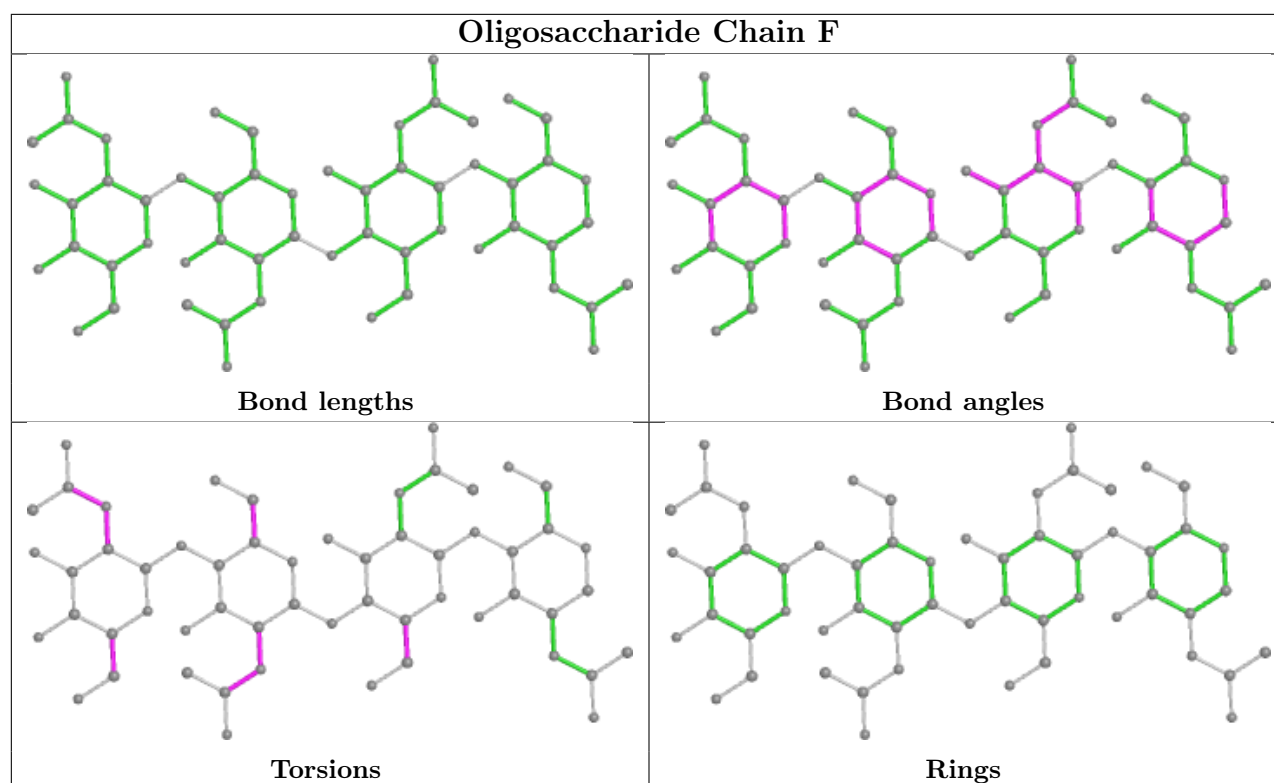












## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	PS1	A	2601	10	36,37,37	1.05	4 (11%)	40,44,44	0.99	2 (5%)
8	CLR	A	2611	-	31,31,31	0.30	0	48,48,48	0.38	0
8	CLR	A	2608	-	31,31,31	0.35	0	48,48,48	0.57	0
8	CLR	A	2612	-	31,31,31	0.33	0	48,48,48	0.55	0
8	CLR	A	2602	-	31,31,31	1.27	5 (16%)	48,48,48	3.08	21 (43%)
11	NAG	A	2605	1	14,14,15	0.35	0	17,19,21	1.33	3 (17%)
13	3PE	A	2614	-	50,50,50	0.29	0	53,55,55	0.33	0
11	NAG	B	1202	2	14,14,15	0.47	0	17,19,21	1.22	2 (11%)
8	CLR	A	2607	-	31,31,31	0.31	0	48,48,48	0.46	0
9	PT5	A	2603	-	64,64,69	0.86	2 (3%)	78,82,87	1.26	7 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	Y01	A	2610	-	38,38,38	0.45	0	57,57,57	0.48	0
13	3PE	A	2613	-	39,39,50	0.35	0	42,44,55	0.36	0
12	Y01	A	2609	-	38,38,38	0.45	0	57,57,57	0.66	0
12	Y01	A	2606	-	38,38,38	0.46	0	57,57,57	0.51	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
7	PS1	A	2601	10	-	22/43/43/43	-
8	CLR	A	2611	-	-	9/10/68/68	0/4/4/4
8	CLR	A	2608	-	-	10/10/68/68	0/4/4/4
8	CLR	A	2612	-	-	9/10/68/68	0/4/4/4
8	CLR	A	2602	-	-	6/10/68/68	0/4/4/4
11	NAG	A	2605	1	-	1/6/23/26	0/1/1/1
13	3PE	A	2614	-	-	16/54/54/54	-
11	NAG	B	1202	2	-	4/6/23/26	0/1/1/1
8	CLR	A	2607	-	-	6/10/68/68	0/4/4/4
9	PT5	A	2603	-	-	26/61/85/90	0/1/1/1
12	Y01	A	2610	-	-	13/19/77/77	0/4/4/4
13	3PE	A	2613	-	-	25/43/43/54	-
12	Y01	A	2609	-	-	10/19/77/77	0/4/4/4
12	Y01	A	2606	-	-	8/19/77/77	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2603	PT5	O18-C11	4.27	1.45	1.33
9	A	2603	PT5	O16-C10	3.75	1.44	1.34
8	A	2602	CLR	C13-C14	-3.18	1.48	1.55
8	A	2602	CLR	C8-C14	-2.76	1.48	1.53
8	A	2602	CLR	C10-C9	-2.47	1.51	1.56
7	A	2601	PS1	O7-C7	2.45	1.40	1.33
7	A	2601	PS1	O9-C5	-2.34	1.40	1.46
7	A	2601	PS1	O9-C17	2.18	1.40	1.34
8	A	2602	CLR	C19-C10	-2.16	1.50	1.54
8	A	2602	CLR	C15-C14	-2.14	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2601	PS1	O7-C6	-2.08	1.40	1.45

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2602	CLR	C14-C8-C9	-12.13	92.85	109.09
8	A	2602	CLR	C19-C10-C9	-7.52	102.72	111.68
8	A	2602	CLR	C1-C10-C9	5.82	116.86	108.73
8	A	2602	CLR	C19-C10-C5	5.24	116.82	108.34
8	A	2602	CLR	C8-C7-C6	-4.74	105.92	112.73
9	A	2603	PT5	O16-C10-C12	4.12	120.39	111.50
8	A	2602	CLR	C12-C11-C9	3.98	120.02	113.11
11	B	1202	NAG	O5-C1-C2	-3.98	105.01	111.29
8	A	2602	CLR	C2-C1-C10	-3.87	104.37	112.74
8	A	2602	CLR	C13-C14-C8	-3.84	108.70	114.38
7	A	2601	PS1	O9-C17-C18	3.83	119.75	111.50
8	A	2602	CLR	C1-C10-C5	-3.79	101.81	108.75
8	A	2602	CLR	C16-C15-C14	-3.70	97.80	105.13
11	A	2605	NAG	C1-C2-N2	3.34	116.19	110.49
9	A	2603	PT5	C5-C6-C1	3.29	115.79	108.96
8	A	2602	CLR	C1-C2-C3	3.20	114.57	110.47
9	A	2603	PT5	O4-C4-C3	3.02	115.69	108.66
9	A	2603	PT5	C2-C3-C4	2.93	116.36	109.68
8	A	2602	CLR	C15-C14-C13	2.78	107.19	103.84
9	A	2603	PT5	C12-C13-C14	-2.72	108.39	113.23
8	A	2602	CLR	C11-C9-C8	-2.70	107.87	111.75
8	A	2602	CLR	C12-C13-C14	-2.59	103.26	107.27
9	A	2603	PT5	O18-C11-C31	2.59	120.02	111.91
11	A	2605	NAG	C2-N2-C7	-2.58	119.24	122.90
8	A	2602	CLR	C18-C13-C14	-2.54	106.97	111.71
8	A	2602	CLR	C4-C5-C10	2.52	119.77	116.42
7	A	2601	PS1	O7-C7-C8	2.43	119.53	111.91
8	A	2602	CLR	C16-C17-C20	-2.41	108.42	112.15
8	A	2602	CLR	C19-C10-C1	-2.29	105.81	109.43
8	A	2602	CLR	C9-C10-C5	2.27	113.21	109.65
11	A	2605	NAG	C3-C4-C5	2.22	114.19	110.24
9	A	2603	PT5	C2-C1-C6	2.20	114.02	110.85
8	A	2602	CLR	C4-C5-C6	-2.17	117.49	120.61
8	A	2602	CLR	C7-C8-C9	2.16	112.33	109.71
11	B	1202	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.



All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2601	PS1	C4-O6-P1-O1
7	A	2601	PS1	C4-O6-P1-O2
8	A	2611	CLR	C13-C17-C20-C21
8	A	2611	CLR	C16-C17-C20-C22
9	A	2603	PT5	C7-O13-P1-O11
9	A	2603	PT5	C1-O1-P1-O12
9	A	2603	PT5	C3-C4-O4-P4
9	A	2603	PT5	C6-C5-O5-P5
9	A	2603	PT5	C4-C5-O5-P5
9	A	2603	PT5	C12-C10-O16-C8
9	A	2603	PT5	C16-C17-C18-C19
12	A	2606	Y01	OAG-CAY-OAW-CBC
12	A	2606	Y01	CAM-CAY-OAW-CBC
12	A	2610	Y01	CAR-CBC-OAW-CAY
12	A	2610	Y01	CAM-CAY-OAW-CBC
13	A	2613	3PE	C1-O11-P-O12
13	A	2613	3PE	C1-O11-P-O13
13	A	2613	3PE	C11-O13-P-O12
13	A	2613	3PE	O21-C2-C3-O31
13	A	2614	3PE	O13-C11-C12-N
13	A	2614	3PE	C22-C21-O21-C2
9	A	2603	PT5	O19-C11-O18-C9
8	A	2611	CLR	C16-C17-C20-C21
12	A	2609	Y01	CAC-CBB-CBE-CAP
12	A	2609	Y01	CAC-CBB-CBE-CBI
8	A	2611	CLR	C13-C17-C20-C22
7	A	2601	PS1	O10-C17-O9-C5
9	A	2603	PT5	O17-C10-O16-C8
13	A	2614	3PE	O22-C21-O21-C2
9	A	2603	PT5	C31-C11-O18-C9
7	A	2601	PS1	C18-C17-O9-C5
8	A	2607	CLR	C21-C20-C22-C23
8	A	2608	CLR	C21-C20-C22-C23
8	A	2611	CLR	C21-C20-C22-C23
8	A	2612	CLR	C21-C20-C22-C23
8	A	2608	CLR	C16-C17-C20-C21
8	A	2612	CLR	C16-C17-C20-C21
8	A	2612	CLR	C13-C17-C20-C21
8	A	2608	CLR	C13-C17-C20-C22
8	A	2612	CLR	C13-C17-C20-C22
12	A	2609	Y01	CAO-CBB-CBE-CBI
12	A	2606	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
12	A	2610	Y01	OAG-CAY-OAW-CBC
8	A	2608	CLR	C13-C17-C20-C21
8	A	2612	CLR	C16-C17-C20-C22
12	A	2609	Y01	CAO-CBB-CBE-CAP
13	A	2613	3PE	C3B-C3C-C3D-C3E
13	A	2613	3PE	C22-C23-C24-C25
12	A	2610	Y01	CAO-CBB-CBE-CBI
8	A	2602	CLR	C17-C20-C22-C23
13	A	2614	3PE	C28-C29-C2A-C2B
11	B	1202	NAG	C8-C7-N2-C2
8	A	2608	CLR	C16-C17-C20-C22
8	A	2611	CLR	C17-C20-C22-C23
12	A	2610	Y01	CAJ-CAO-CBB-CBE
13	A	2613	3PE	C32-C33-C34-C35
7	A	2601	PS1	C8-C7-O7-C6
12	A	2610	Y01	CAC-CBB-CBE-CBI
9	A	2603	PT5	C1-O1-P1-O13
8	A	2608	CLR	C17-C20-C22-C23
8	A	2612	CLR	C17-C20-C22-C23
11	B	1202	NAG	O7-C7-N2-C2
8	A	2608	CLR	C22-C23-C24-C25
7	A	2601	PS1	C17-C18-C19-C20
8	A	2607	CLR	C22-C23-C24-C25
12	A	2606	Y01	CAN-CAJ-CAO-CBB
13	A	2614	3PE	C24-C25-C26-C27
8	A	2602	CLR	C21-C20-C22-C23
7	A	2601	PS1	O8-C7-O7-C6
7	A	2601	PS1	C7-C8-C9-C10
9	A	2603	PT5	C10-C12-C13-C14
12	A	2610	Y01	CAX-CAL-CAM-CAY
8	A	2608	CLR	C20-C22-C23-C24
8	A	2612	CLR	C22-C23-C24-C25
12	A	2610	Y01	CAO-CAJ-CAN-CBA
12	A	2609	Y01	CAJ-CAO-CBB-CBE
7	A	2601	PS1	C1-O3-P1-O6
7	A	2601	PS1	C4-O6-P1-O3
13	A	2613	3PE	C11-O13-P-O11
7	A	2601	PS1	N1-C2-C3-O5
12	A	2610	Y01	CAJ-CAO-CBB-CAC
8	A	2607	CLR	C20-C22-C23-C24
12	A	2606	Y01	CAJ-CAN-CBA-CAB
13	A	2613	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
13	A	2613	3PE	C38-C39-C3A-C3B
8	A	2602	CLR	C22-C23-C24-C25
12	A	2610	Y01	CAC-CBB-CBE-CAP
13	A	2613	3PE	C37-C38-C39-C3A
8	A	2607	CLR	C17-C20-C22-C23
13	A	2613	3PE	C3D-C3E-C3F-C3G
12	A	2609	Y01	CAJ-CAO-CBB-CAC
8	A	2607	CLR	C23-C24-C25-C26
12	A	2606	Y01	CAJ-CAN-CBA-CAA
13	A	2613	3PE	C22-C21-O21-C2
8	A	2608	CLR	C23-C24-C25-C27
8	A	2612	CLR	C23-C24-C25-C26
12	A	2610	Y01	CAO-CBB-CBE-CAP
13	A	2613	3PE	O22-C21-O21-C2
11	B	1202	NAG	O5-C5-C6-O6
8	A	2602	CLR	C23-C24-C25-C26
7	A	2601	PS1	O6-C4-C5-O9
12	A	2606	Y01	CAJ-CAO-CBB-CBE
8	A	2608	CLR	C23-C24-C25-C26
8	A	2612	CLR	C23-C24-C25-C27
9	A	2603	PT5	C11-C31-C32-C33
13	A	2613	3PE	C3F-C3G-C3H-C3I
9	A	2603	PT5	C35-C36-C37-C38
13	A	2614	3PE	O31-C31-C32-C33
11	A	2605	NAG	O5-C5-C6-O6
8	A	2611	CLR	C23-C24-C25-C26
13	A	2613	3PE	C3C-C3D-C3E-C3F
13	A	2613	3PE	C39-C3A-C3B-C3C
9	A	2603	PT5	C1-O1-P1-O11
9	A	2603	PT5	C15-C16-C17-C18
9	A	2603	PT5	C21-C22-C23-C24
12	A	2606	Y01	CAJ-CAO-CBB-CAC
13	A	2613	3PE	C23-C24-C25-C26
8	A	2602	CLR	C23-C24-C25-C27
12	A	2609	Y01	CAL-CAM-CAY-OAW
8	A	2607	CLR	C23-C24-C25-C27
8	A	2611	CLR	C23-C24-C25-C27
7	A	2601	PS1	N1-C2-C3-O4
9	A	2603	PT5	C27-C28-C29-C30
7	A	2601	PS1	O6-C4-C5-C6
7	A	2601	PS1	C6-C5-O9-C17
8	A	2611	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
13	A	2613	3PE	C1-C2-C3-O31
13	A	2614	3PE	O11-C1-C2-O21
12	A	2610	Y01	CAJ-CAN-CBA-CAA
7	A	2601	PS1	C1-O3-P1-O1
13	A	2613	3PE	C1-O11-P-O14
11	B	1202	NAG	C4-C5-C6-O6
7	A	2601	PS1	C22-C23-C24-C25
9	A	2603	PT5	C7-C8-O16-C10
9	A	2603	PT5	C7-O13-P1-O1
13	A	2613	3PE	O31-C31-C32-C33
13	A	2614	3PE	O32-C31-C32-C33
12	A	2610	Y01	CAJ-CAN-CBA-CAB
12	A	2609	Y01	CAN-CAJ-CAO-CBB
13	A	2613	3PE	C35-C36-C37-C38
13	A	2614	3PE	C26-C27-C28-C29
13	A	2614	3PE	C2-C1-O11-P
7	A	2601	PS1	C1-C2-C3-O5
13	A	2614	3PE	C1-C2-O21-C21
9	A	2603	PT5	C18-C19-C20-C21
9	A	2603	PT5	C19-C20-C21-C22
13	A	2614	3PE	C3A-C3B-C3C-C3D
8	A	2602	CLR	C13-C17-C20-C21
13	A	2613	3PE	C24-C25-C26-C27
13	A	2614	3PE	C38-C39-C3A-C3B
7	A	2601	PS1	C20-C21-C22-C23
9	A	2603	PT5	C13-C14-C15-C16
12	A	2609	Y01	CAL-CAM-CAY-OAG
7	A	2601	PS1	O9-C17-C18-C19
9	A	2603	PT5	C12-C13-C14-C15
13	A	2614	3PE	O11-C1-C2-C3
9	A	2603	PT5	C5-O5-P5-O51
7	A	2601	PS1	O3-C1-C2-N1
13	A	2614	3PE	C22-C23-C24-C25
7	A	2601	PS1	O10-C17-C18-C19
13	A	2613	3PE	O13-C11-C12-N
9	A	2603	PT5	O18-C11-C31-C32
13	A	2613	3PE	C12-C11-O13-P
13	A	2614	3PE	C37-C38-C39-C3A
12	A	2609	Y01	CAO-CAJ-CAN-CBA

There are no ring outliers.

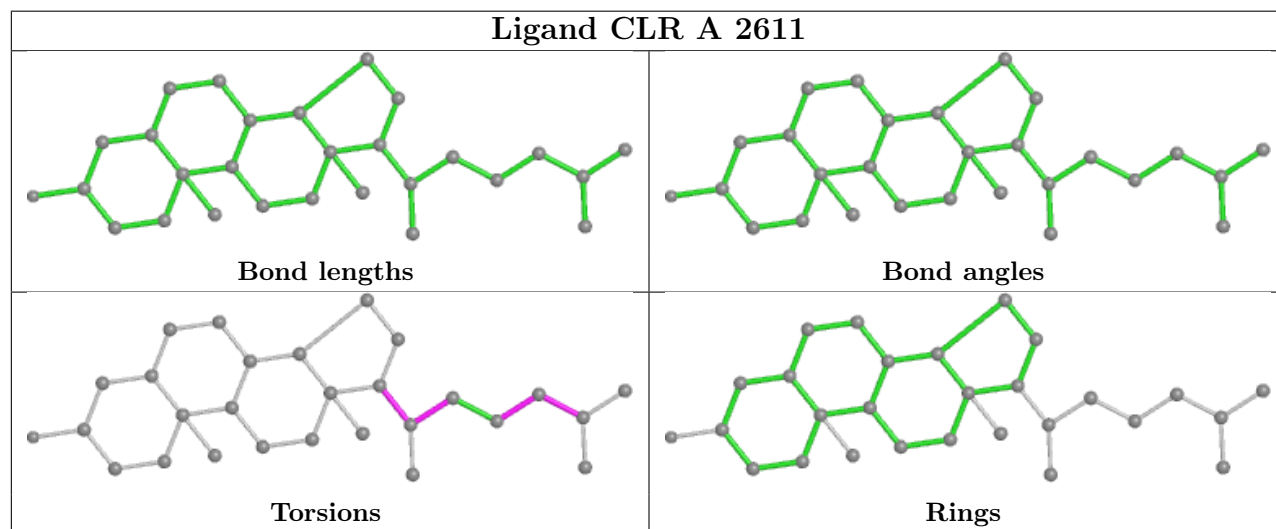
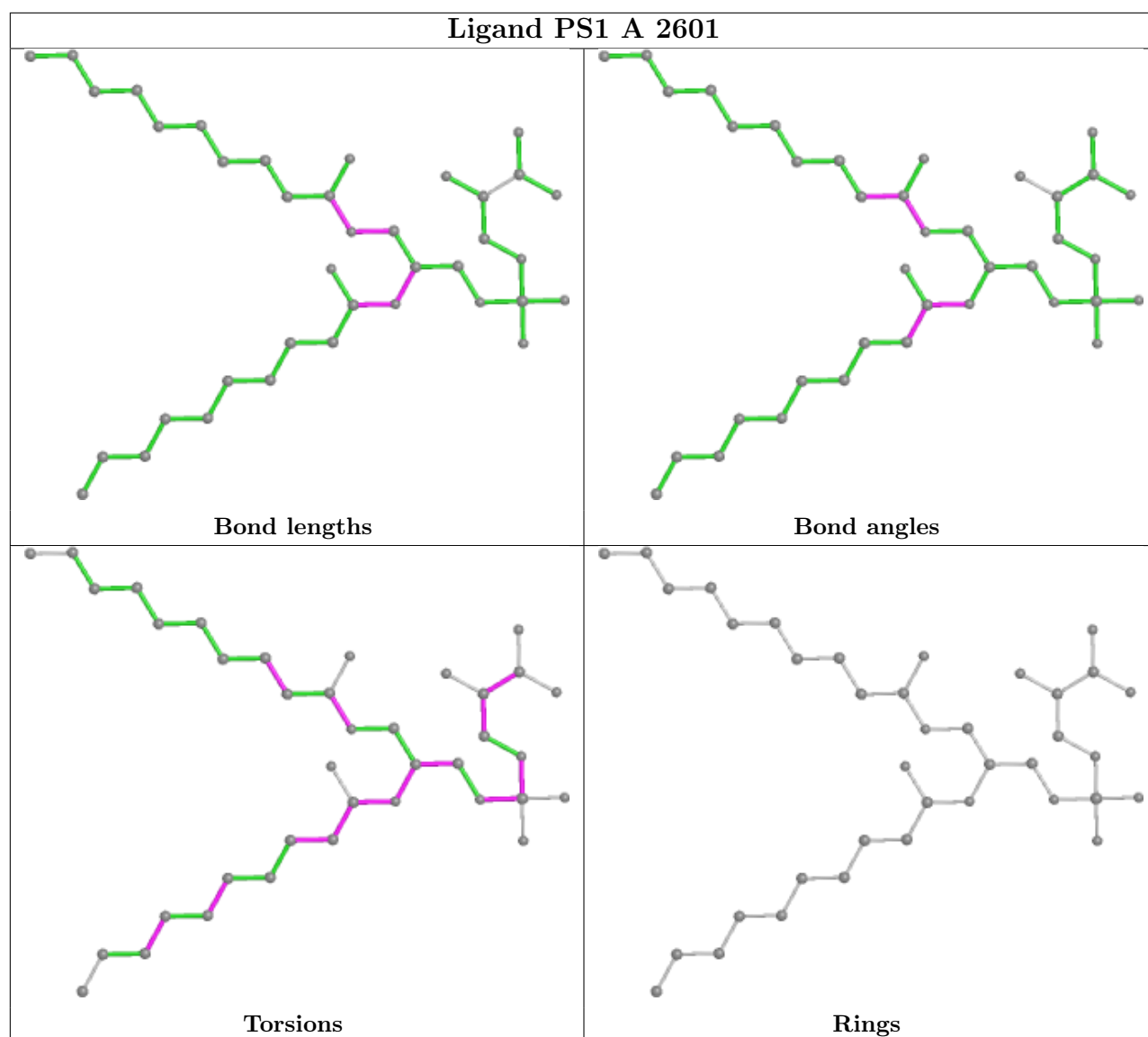
12 monomers are involved in 62 short contacts:



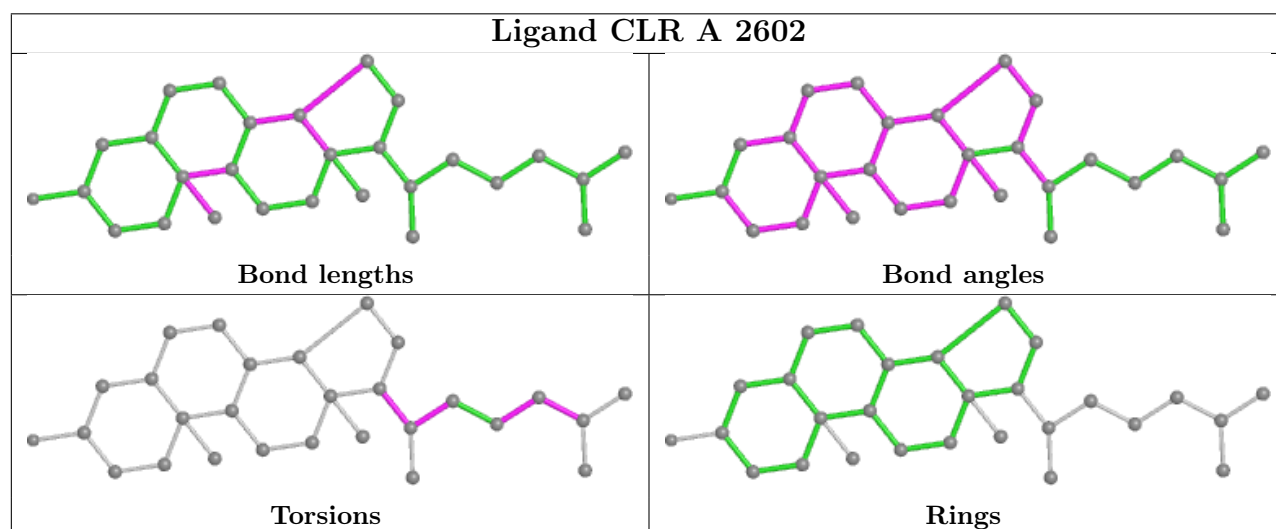
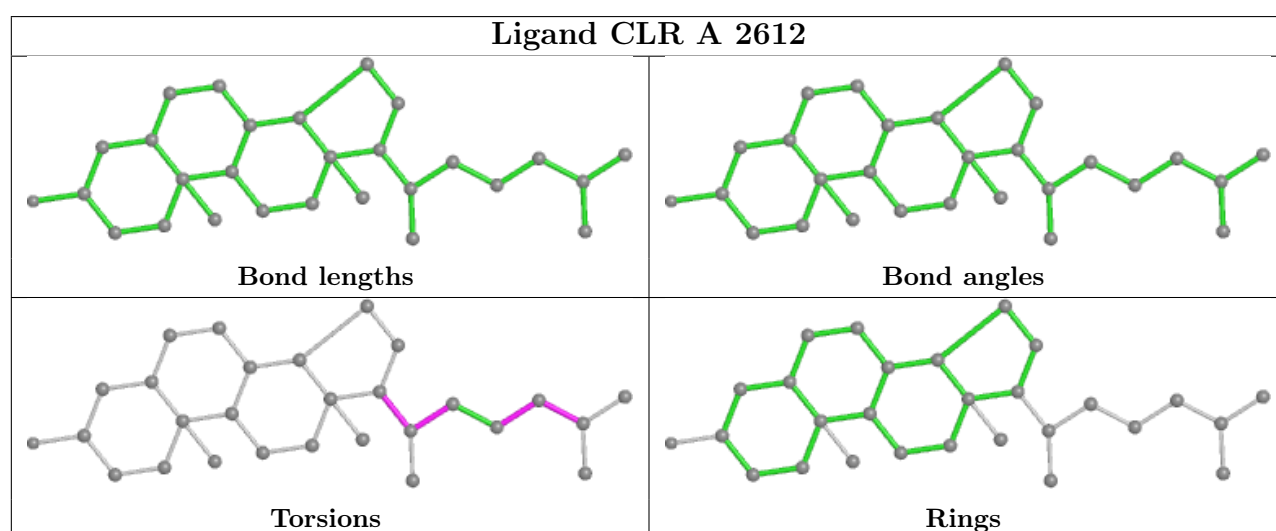
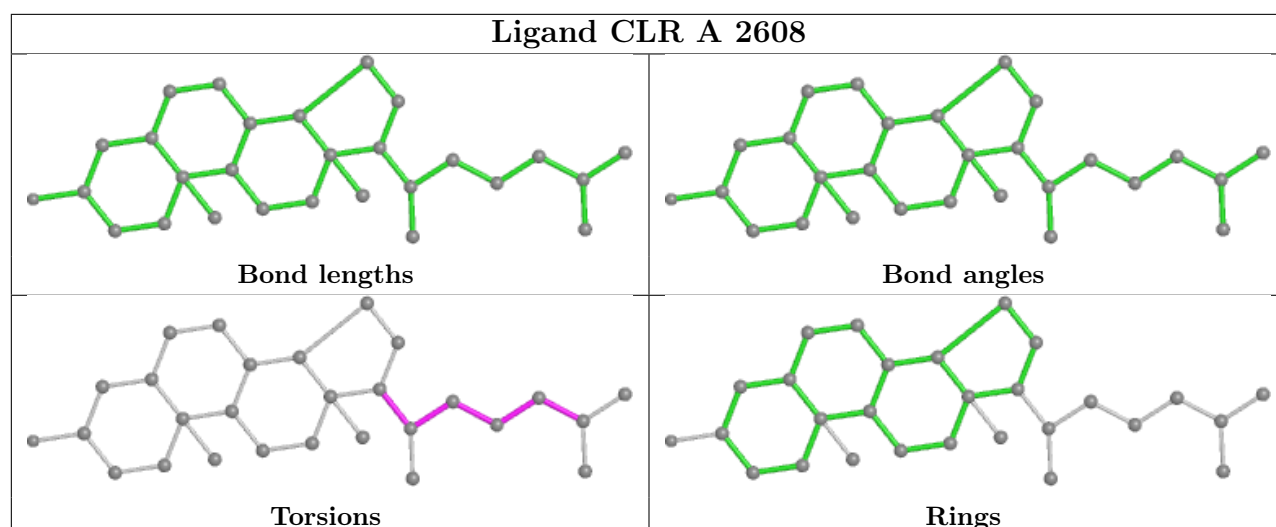
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2601	PS1	3	0
8	A	2611	CLR	5	0
8	A	2608	CLR	6	0
8	A	2612	CLR	1	0
8	A	2602	CLR	7	0
13	A	2614	3PE	6	0
8	A	2607	CLR	1	0
9	A	2603	PT5	4	0
12	A	2610	Y01	5	0
13	A	2613	3PE	9	0
12	A	2609	Y01	8	0
12	A	2606	Y01	11	0

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.

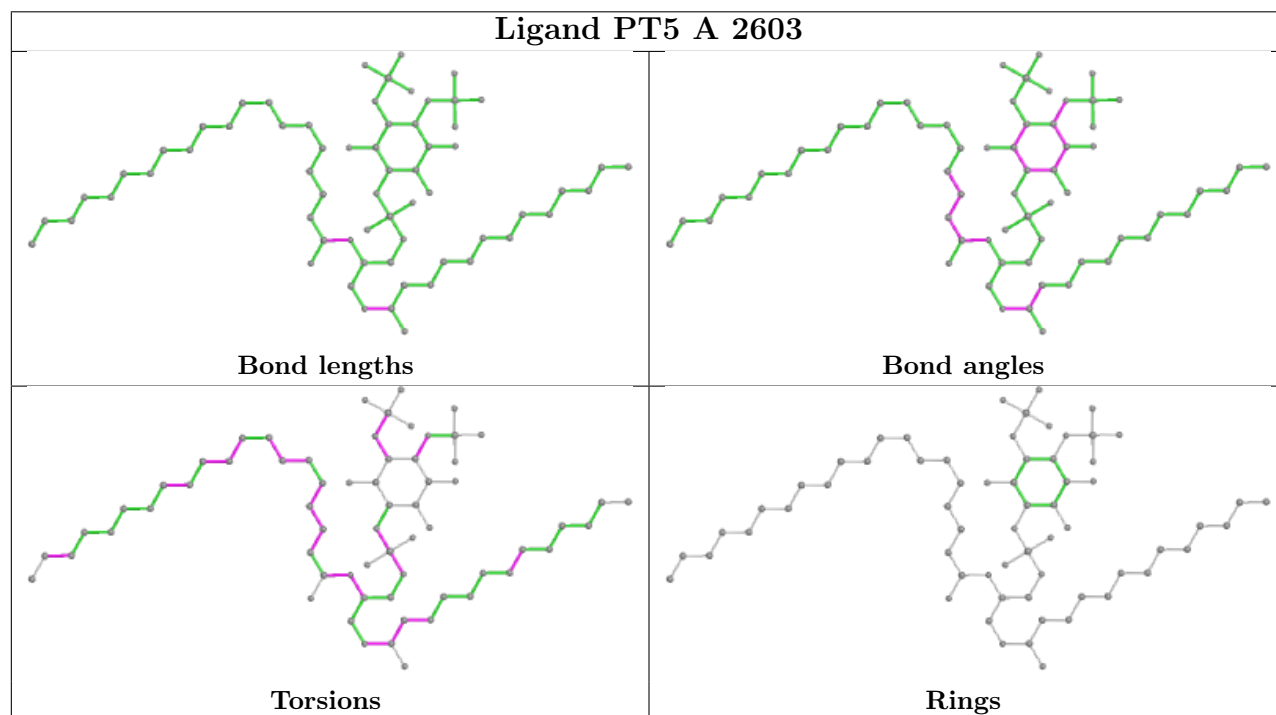
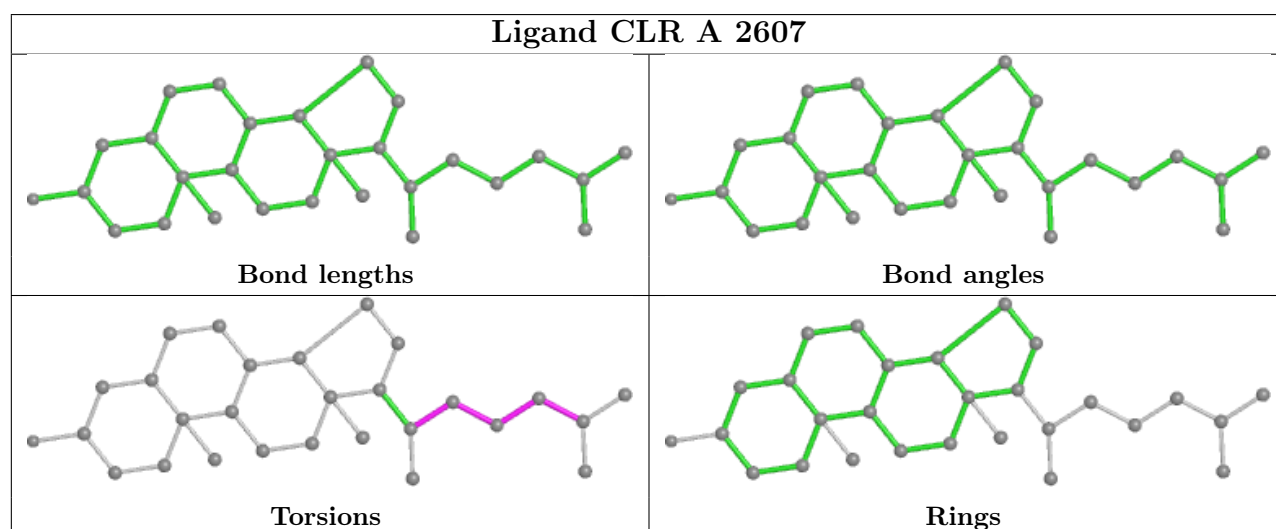
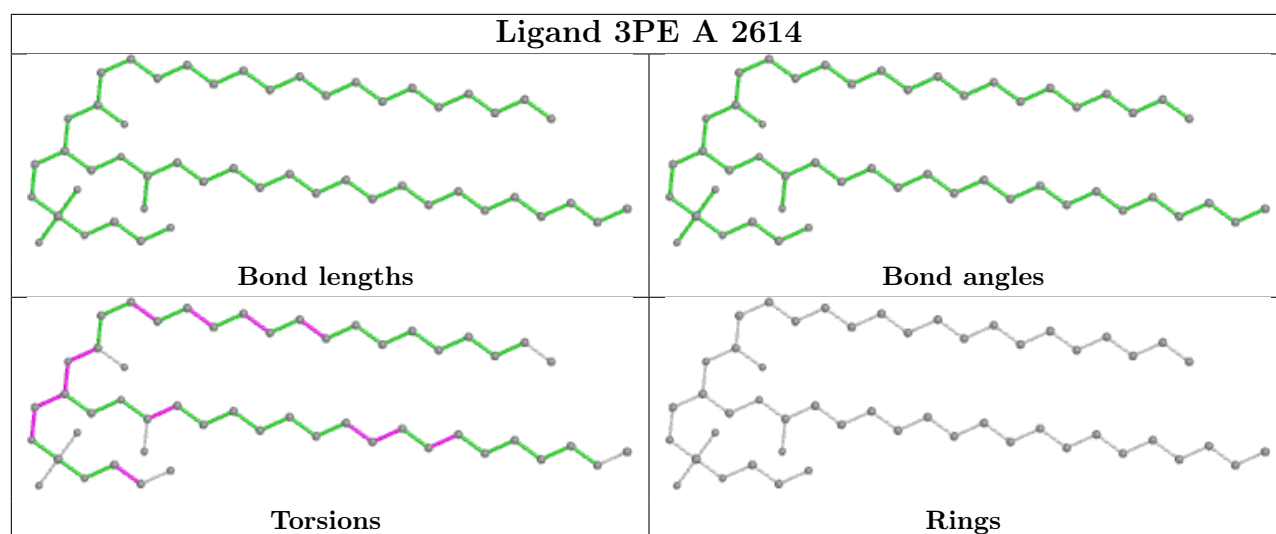




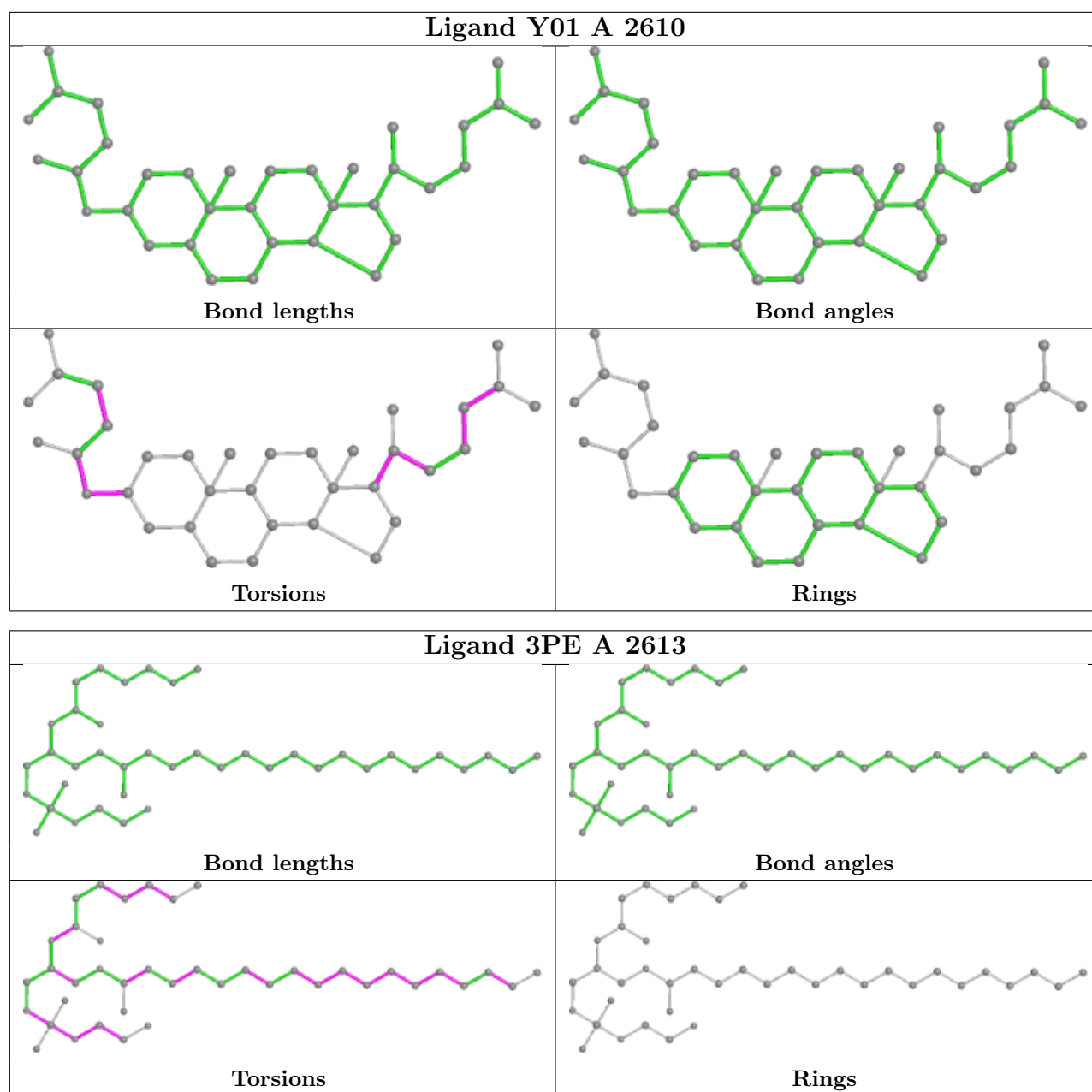




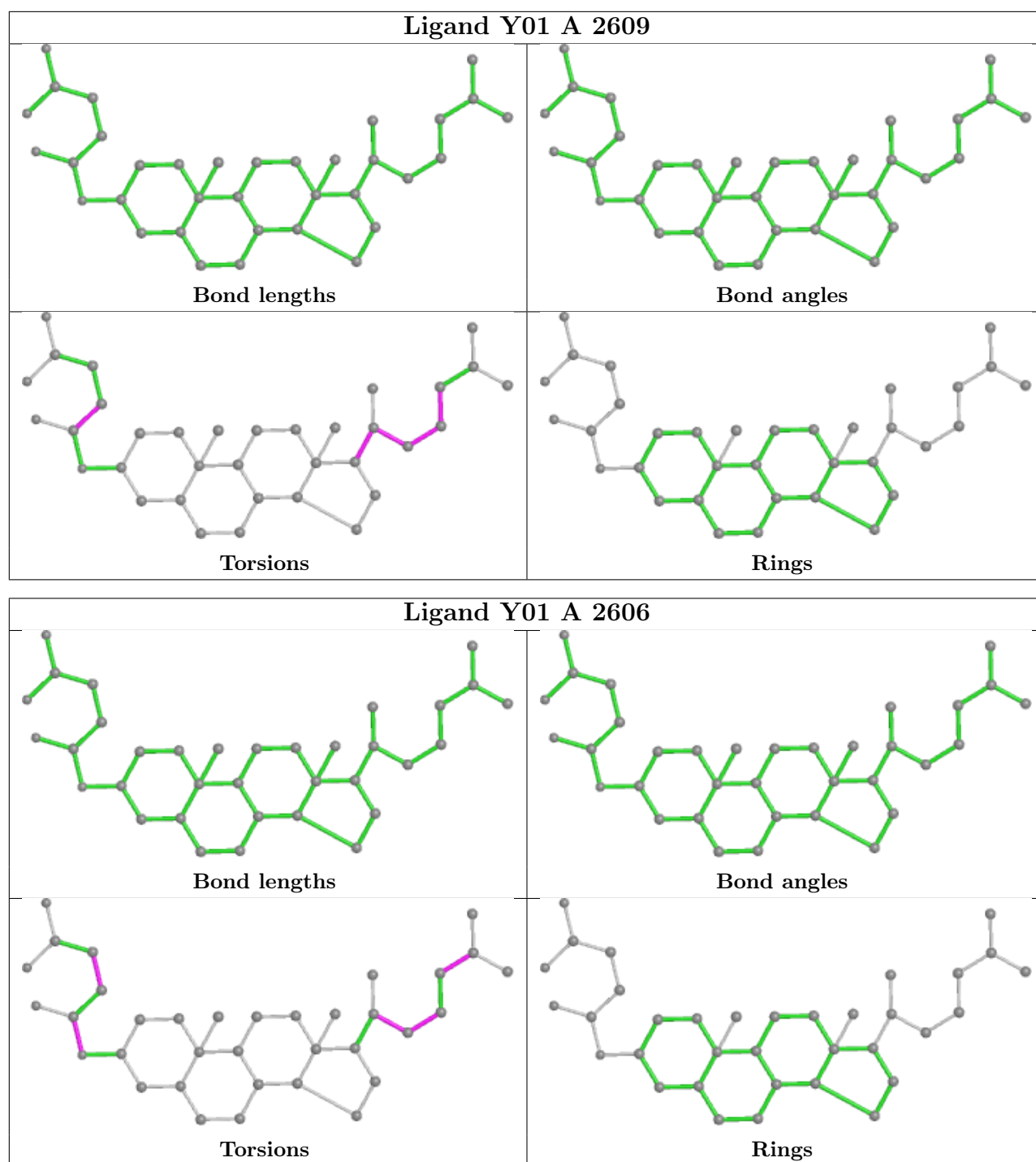












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



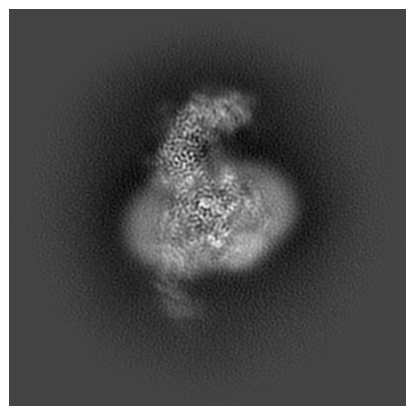
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38158. These allow visual inspection of the internal detail of the map and identification of artifacts.

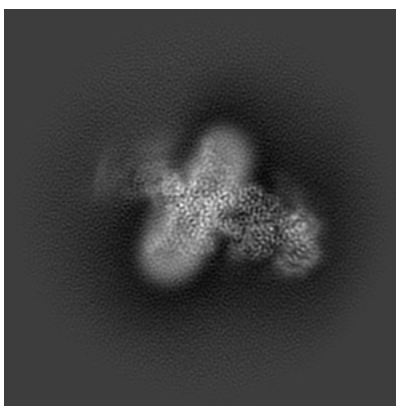
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

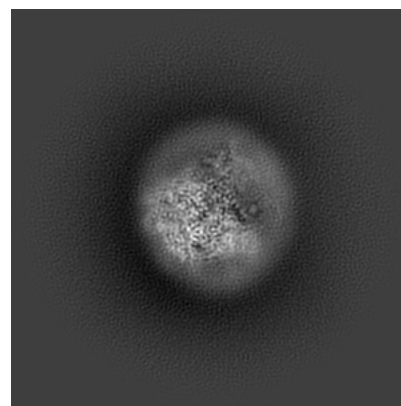
#### 6.1.1 Primary map



X

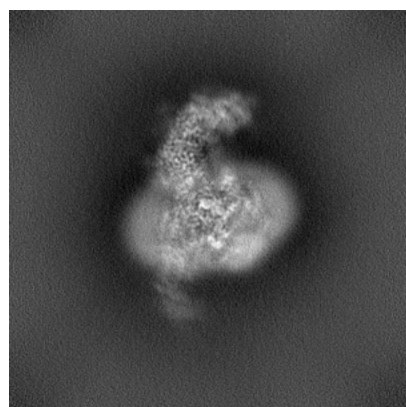


Y

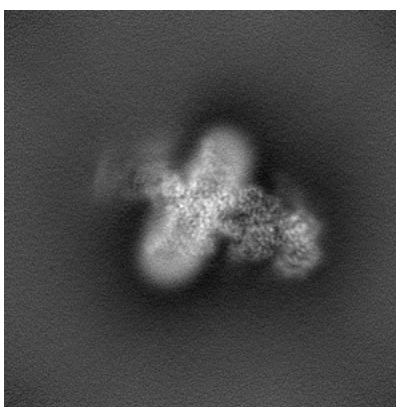


Z

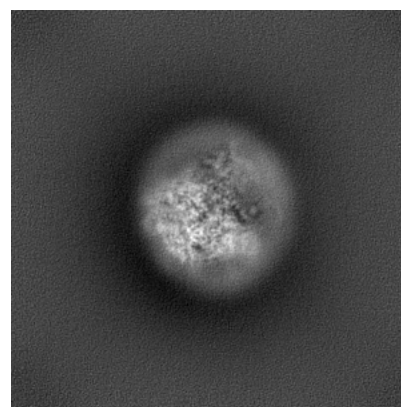
#### 6.1.2 Raw map



X



Y



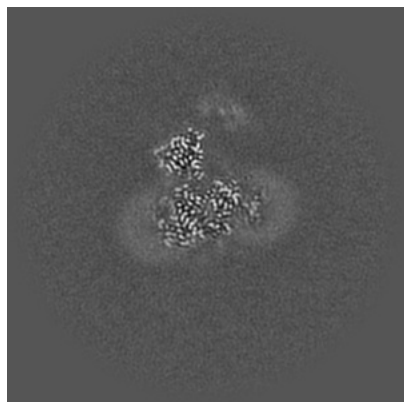
Z

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

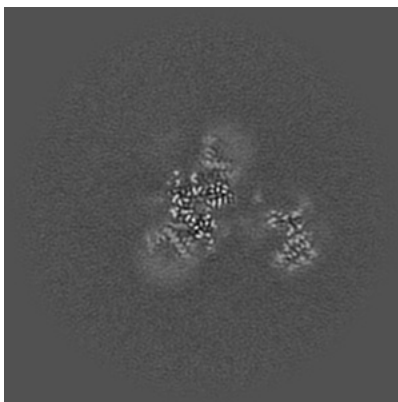


## 6.2 Central slices [i](#)

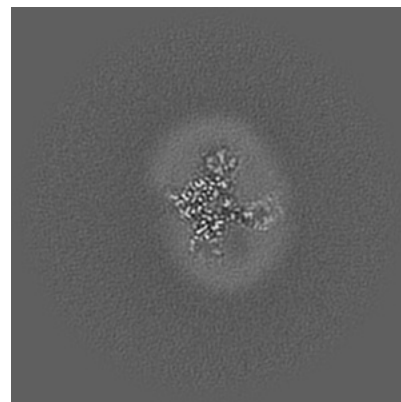
### 6.2.1 Primary map



X Index: 160

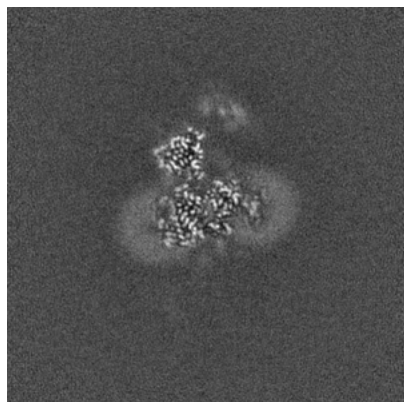


Y Index: 160

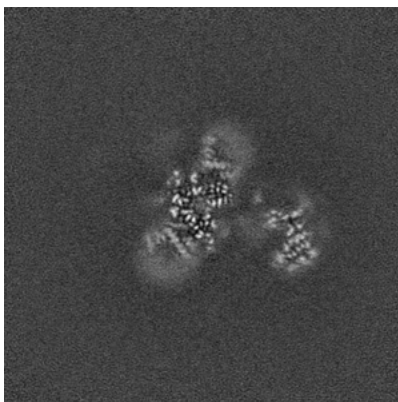


Z Index: 160

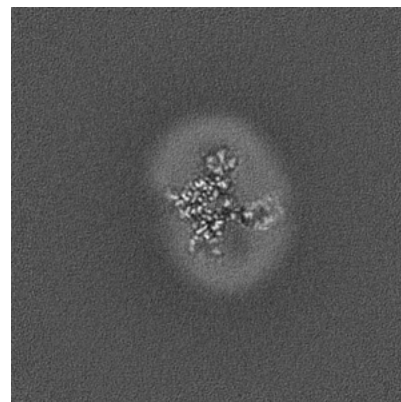
### 6.2.2 Raw map



X Index: 160



Y Index: 160



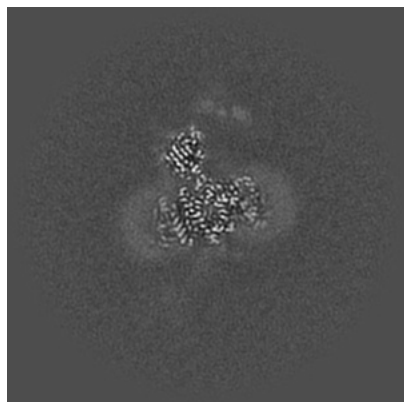
Z Index: 160

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

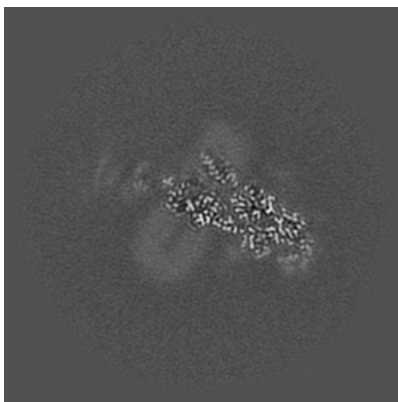


## 6.3 Largest variance slices [i](#)

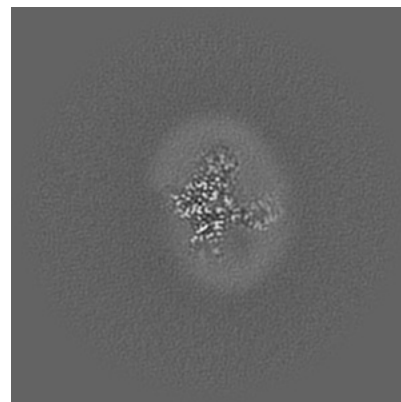
### 6.3.1 Primary map



X Index: 163

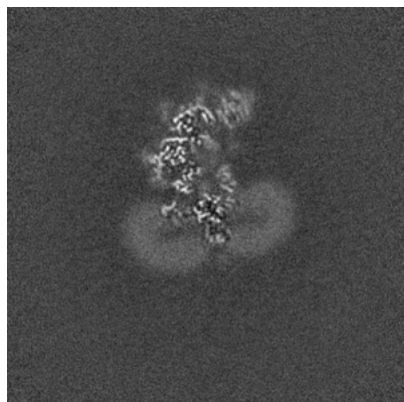


Y Index: 144

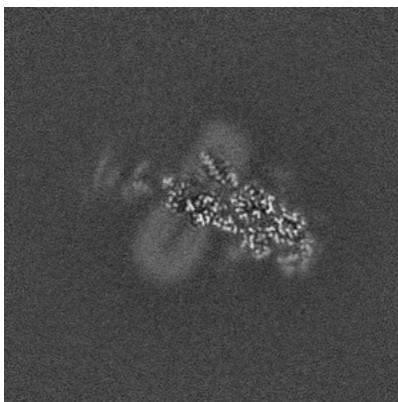


Z Index: 161

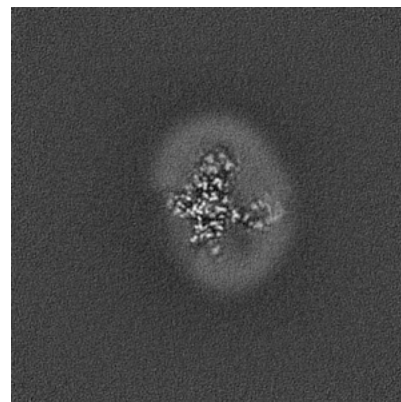
### 6.3.2 Raw map



X Index: 144



Y Index: 144



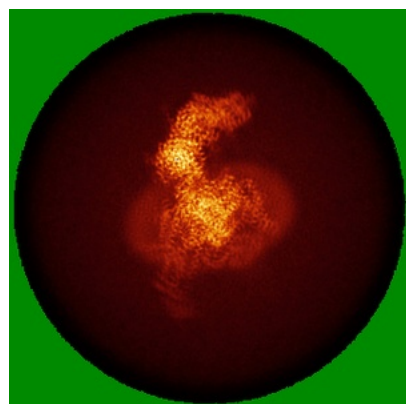
Z Index: 162

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

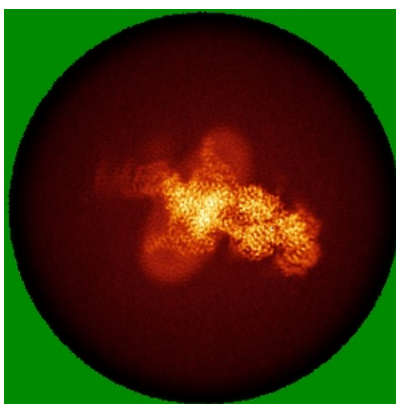


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

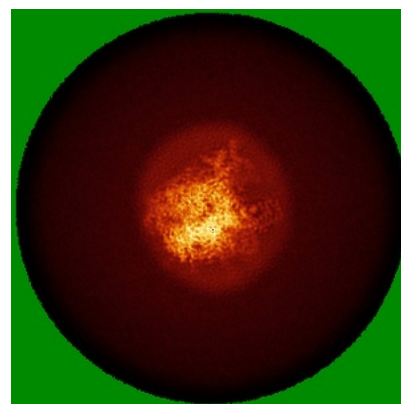
### 6.4.1 Primary map



X

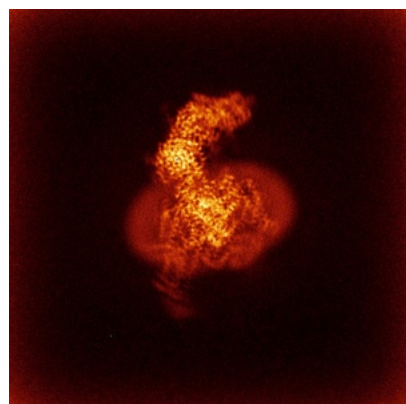


Y

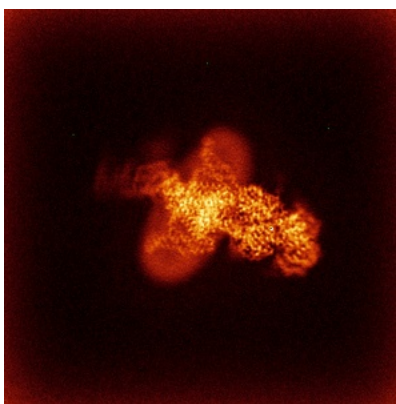


Z

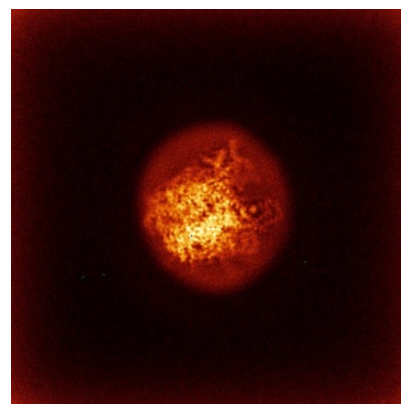
### 6.4.2 Raw map



X



Y



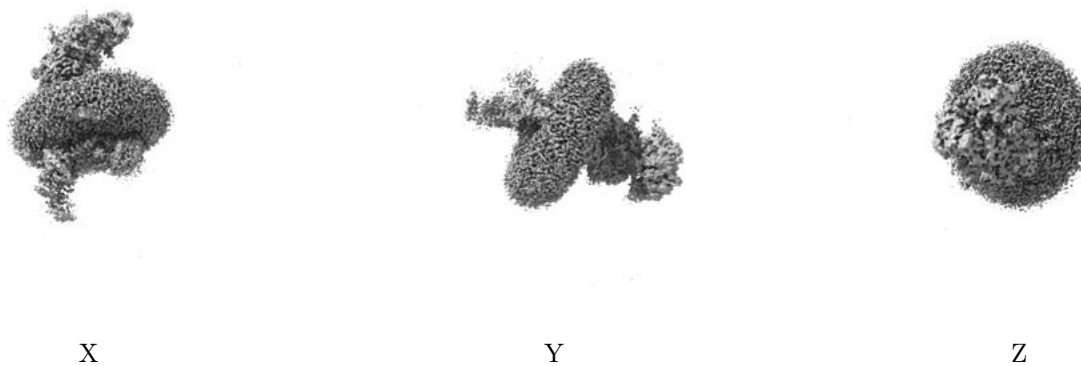
Z

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



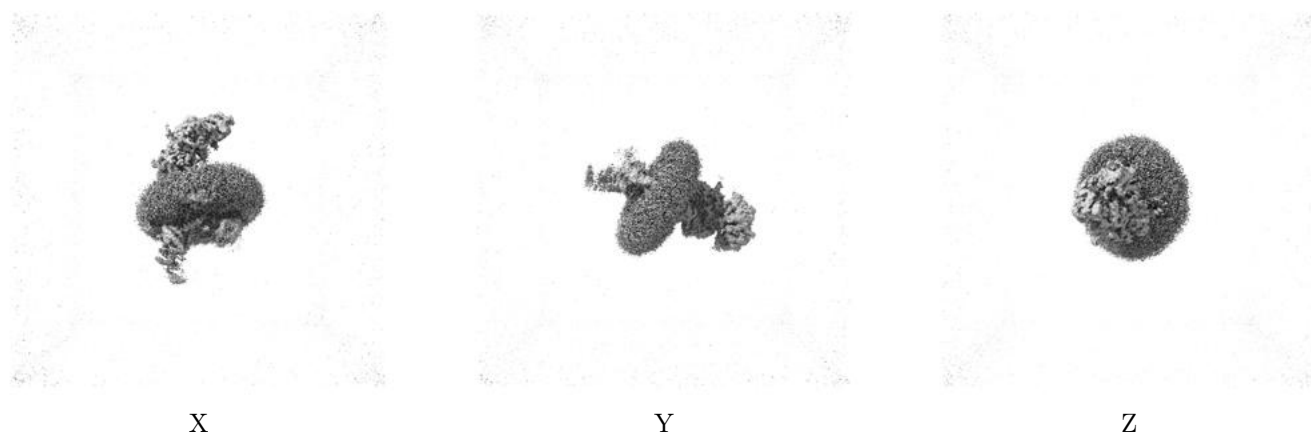
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

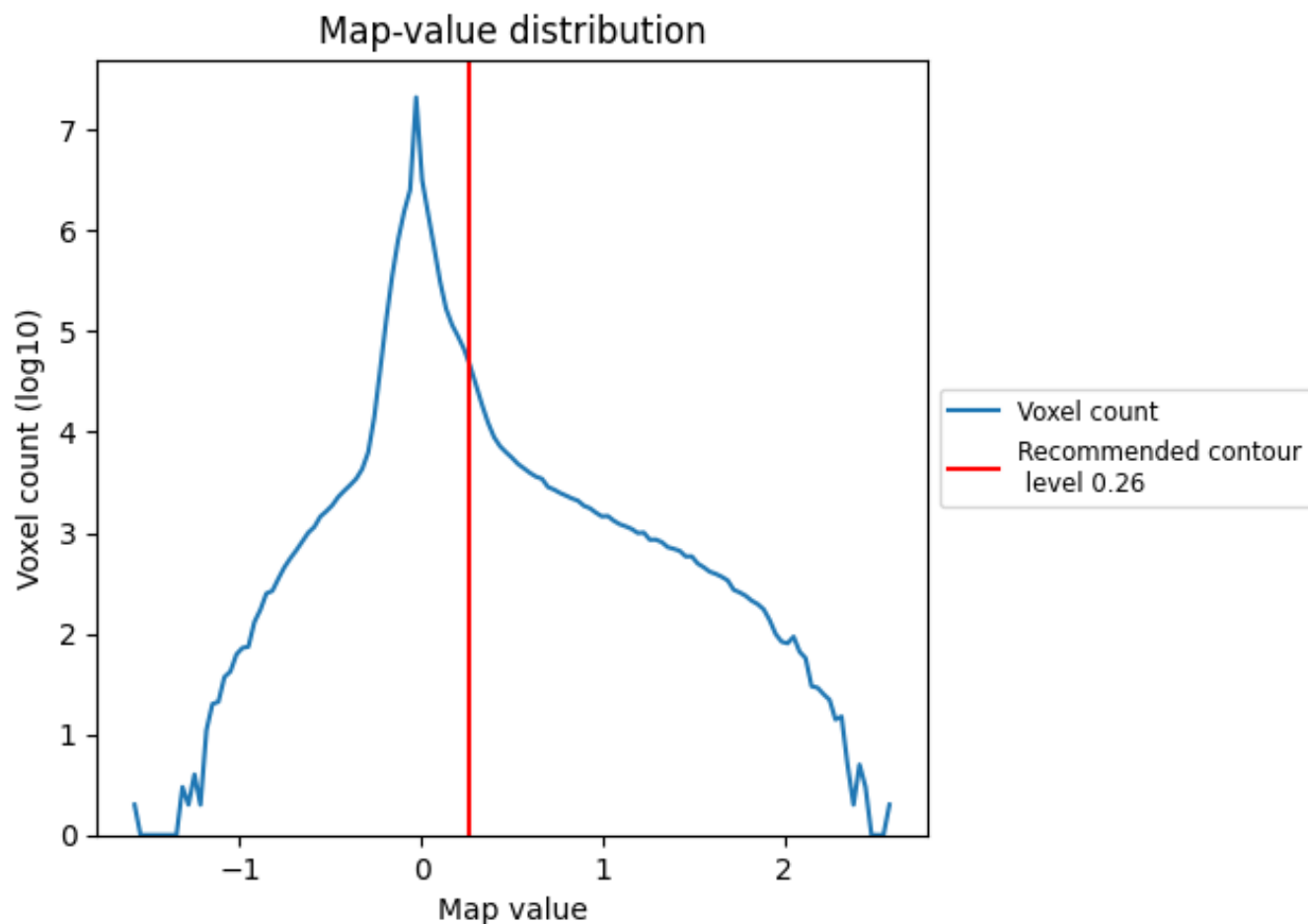
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

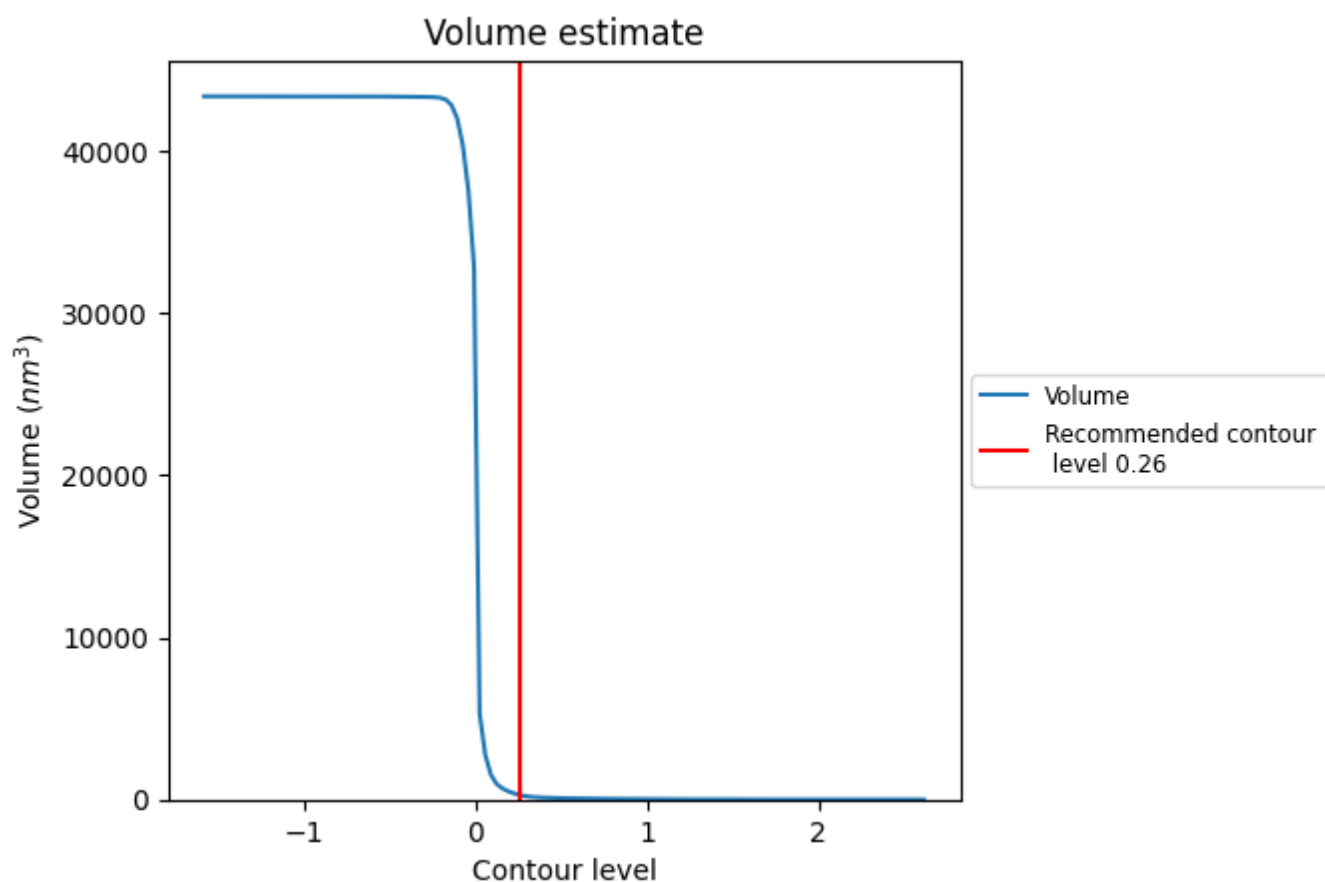
### 7.1 Map-value distribution [i](#)



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](#)

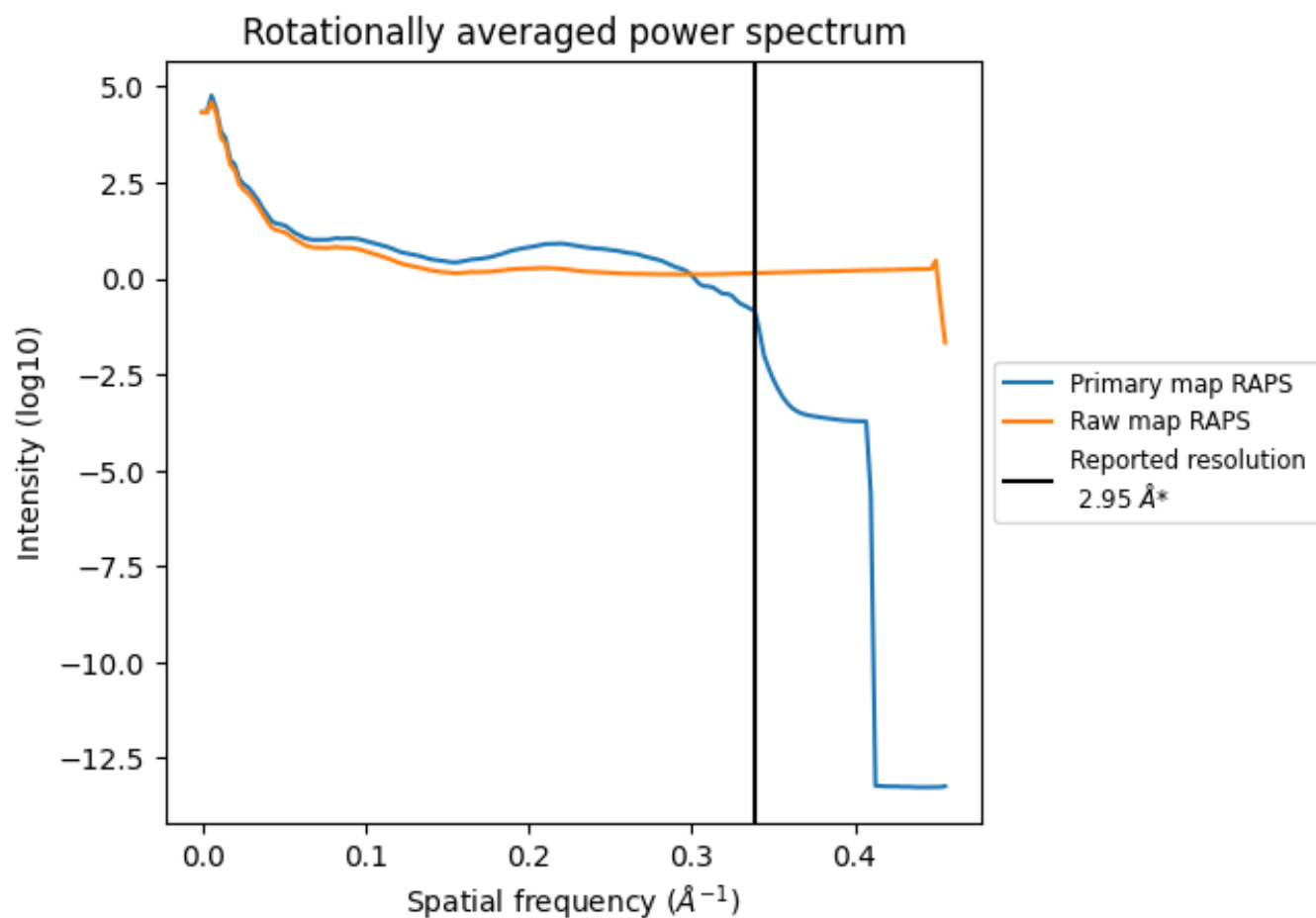


The volume at the recommended contour level is 282 nm<sup>3</sup>; this corresponds to an approximate mass of 255 kDa.

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 ⓘ



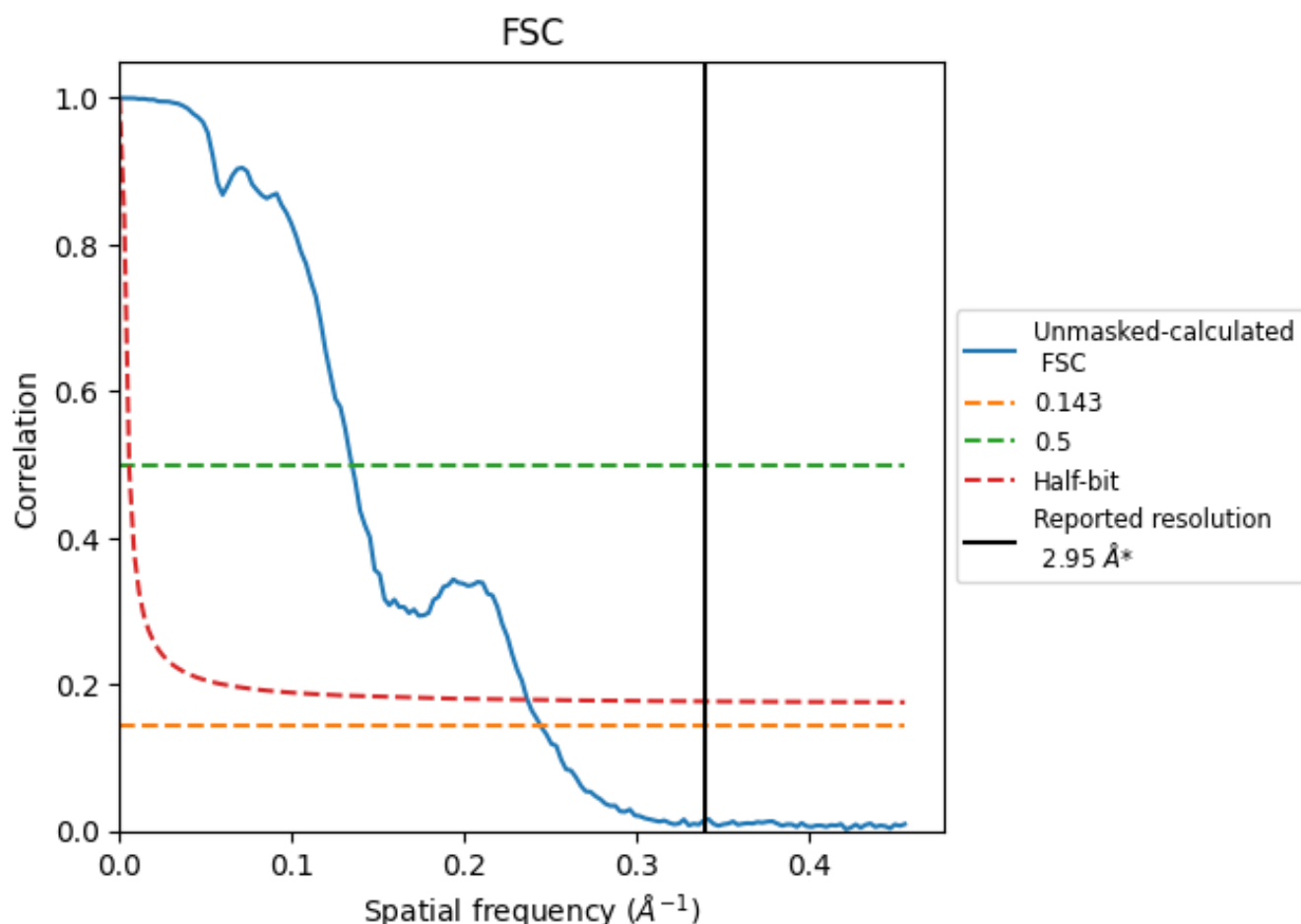
\*Reported resolution corresponds to spatial frequency of 0.339 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.339 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	7.42	4.23

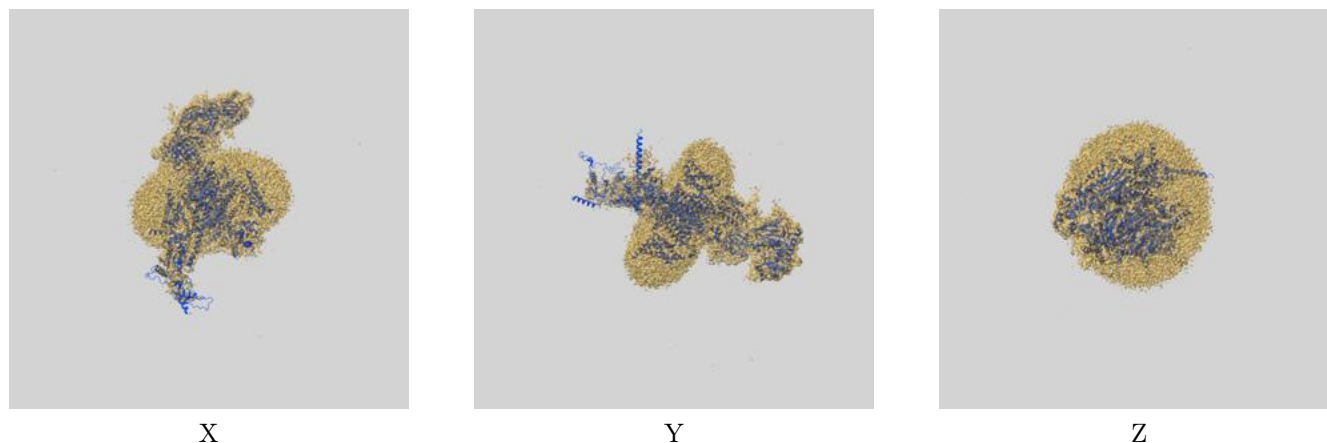
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 2.95 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38158 and PDB model 8X90. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

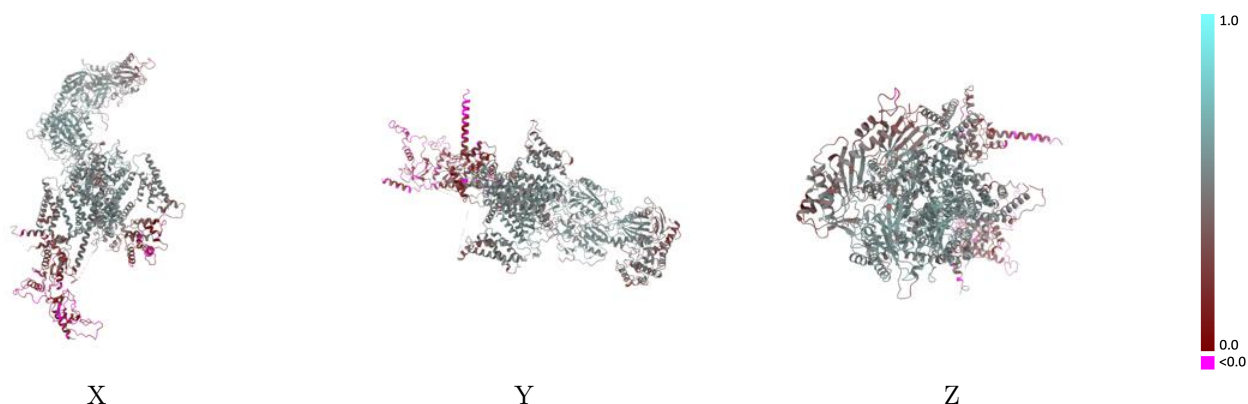
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

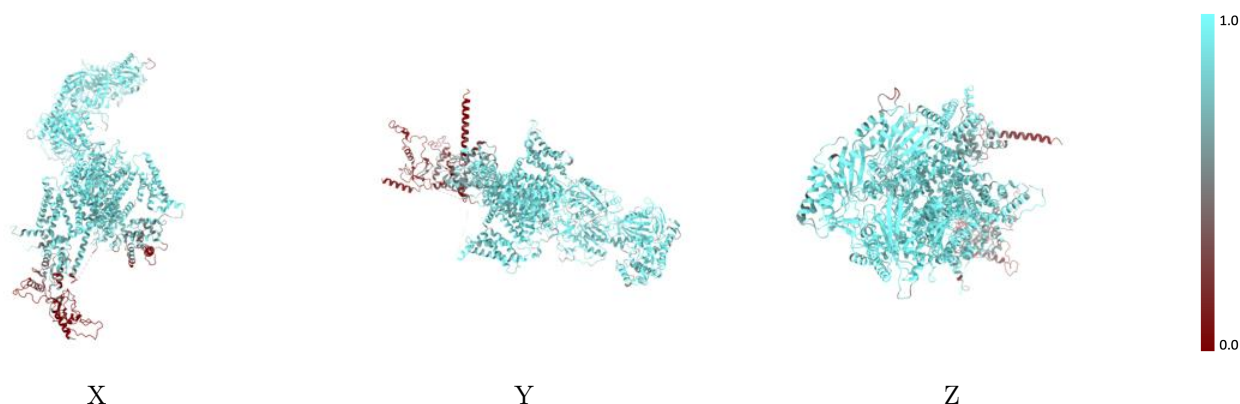


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

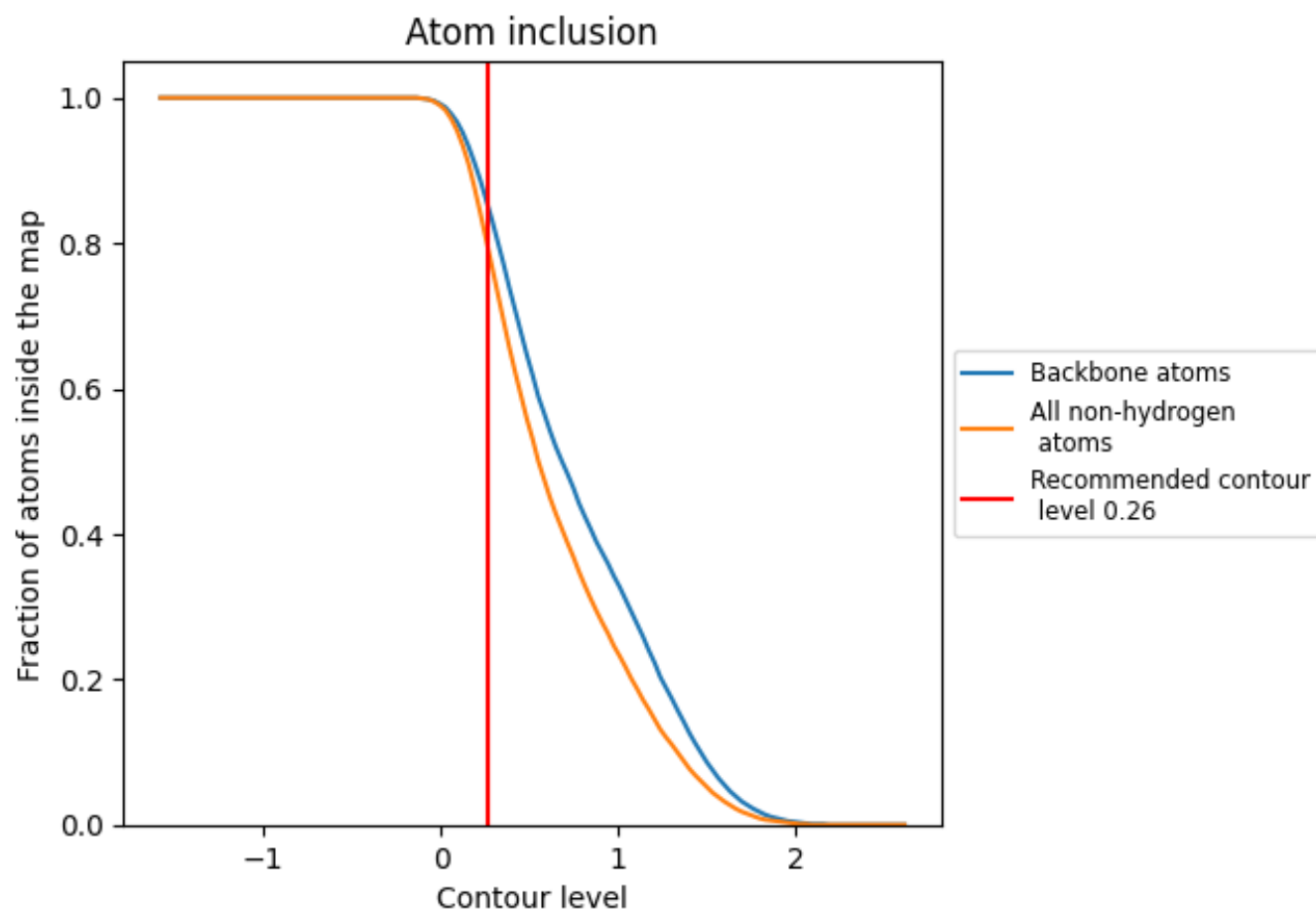
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8010	<div></div> 0.4390
A	<div></div> 0.8320	<div></div> 0.4610
B	<div></div> 0.9120	<div></div> 0.4960
C	<div></div> 0.3210	<div></div> 0.1640
D	<div></div> 0.8810	<div></div> 0.4880
E	<div></div> 0.8210	<div></div> 0.4630
F	<div></div> 0.9640	<div></div> 0.5470
G	<div></div> 0.8570	<div></div> 0.5440
H	<div></div> 0.9290	<div></div> 0.4840

1.0

0.0

<0.0