



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 11:50 PM EDT

PDB ID : 8EPL  
EMDB ID : EMD-28529  
Title : Human R-type voltage-gated calcium channel Cav2.3 at 3.1 Angstrom resolution  
Authors : Gao, S.; Yao, X.; Yan, N.  
Deposited on : 2022-10-06  
Resolution : 3.10 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>.

---

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) : 2.39

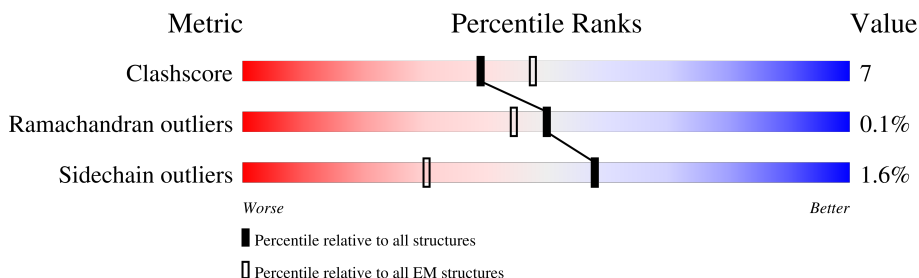
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	2313	
2	B	484	
3	C	1103	
4	D	2	
4	E	2	
4	G	2	
4	H	2	
5	F	4	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20953 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 R-type calcium channel subunit alpha-1E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1274	Total	C	N	O	S	0	0
			10316	6777	1688	1775	76		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

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

cetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

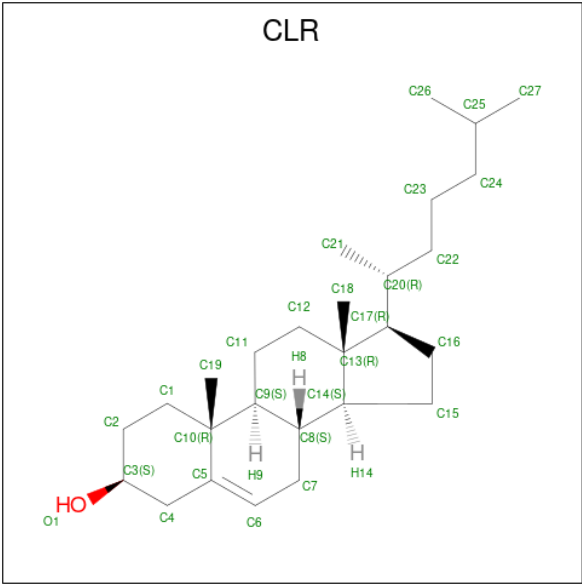


Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



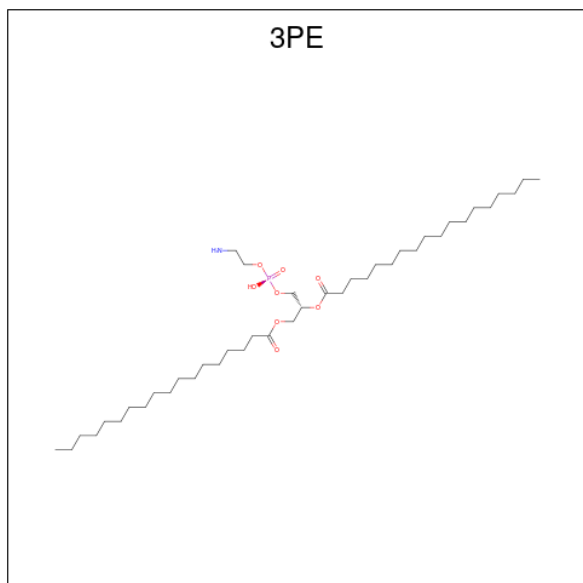
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	

Continued on next page...

Continued from previous page...

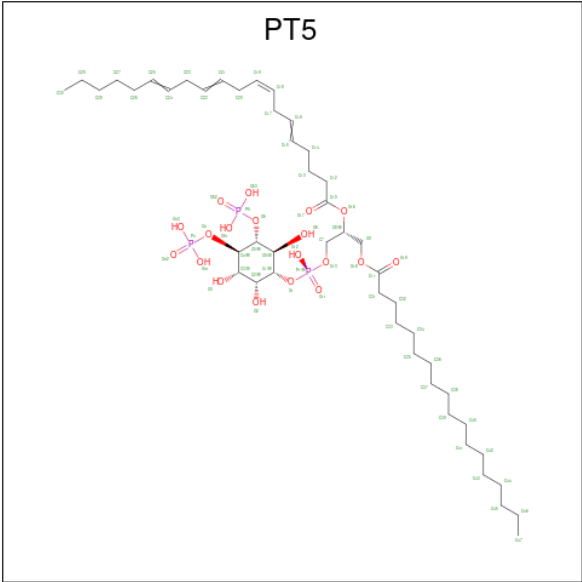
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



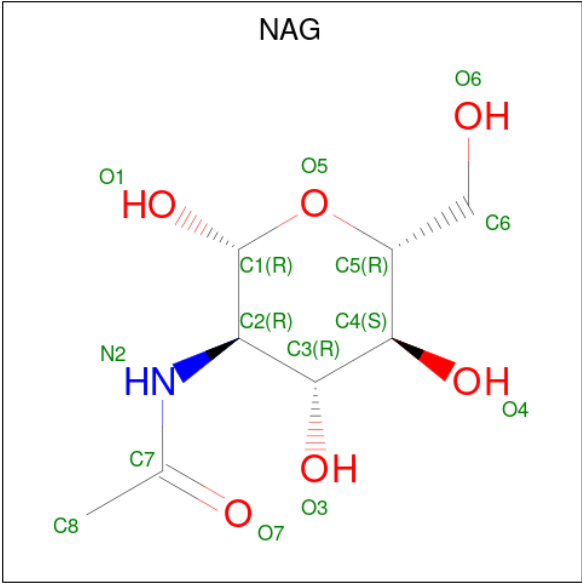
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	A	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 9 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]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 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
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

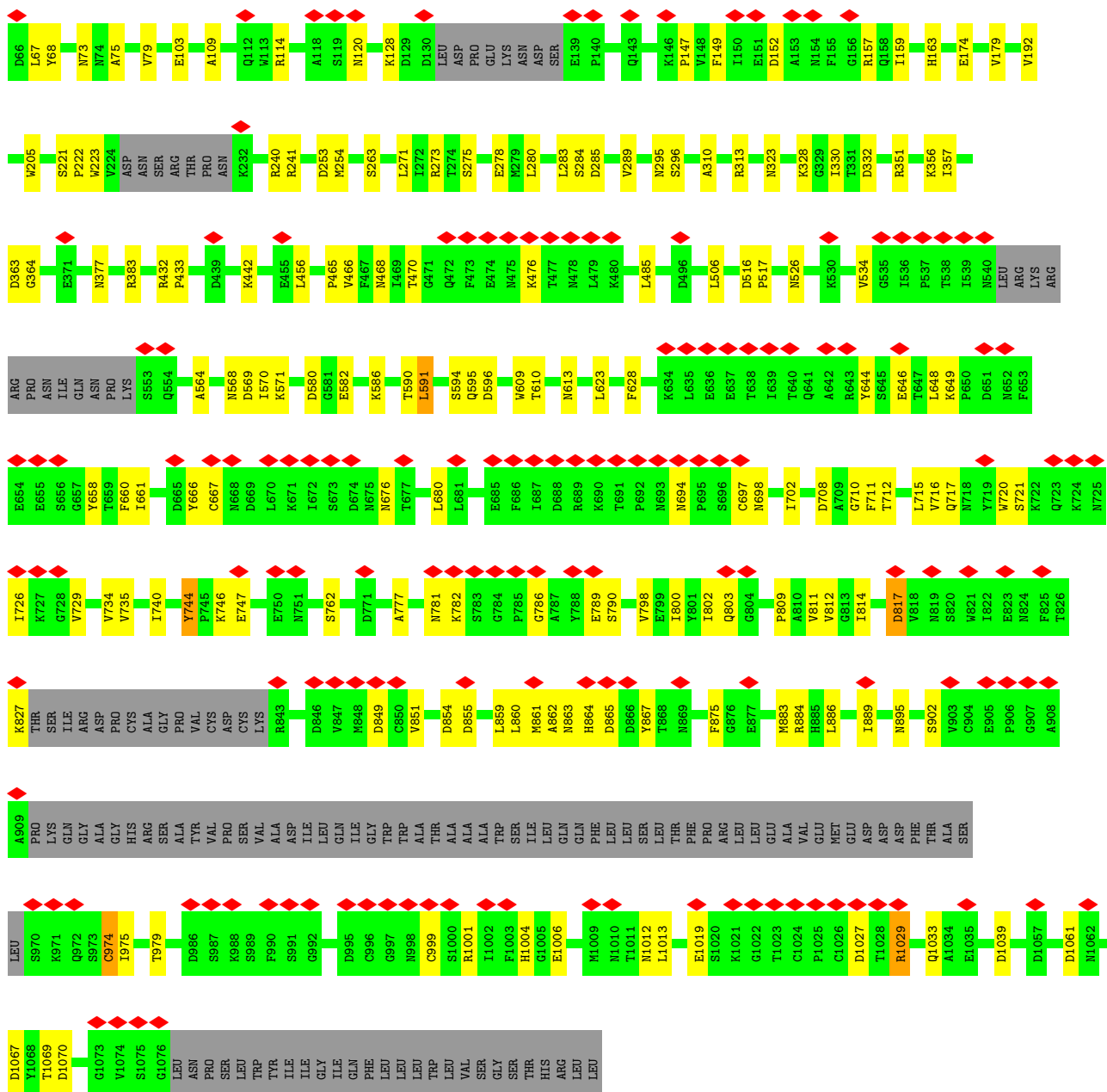
*Continued from previous page...*

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









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



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





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



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



- Molecule 5: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118244	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)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CLR, NAG, 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	0.25	0/10565	0.45	0/14299
2	B	0.24	0/2624	0.49	0/3544
3	C	0.26	0/7728	0.47	0/10477
All	All	0.25	0/20917	0.46	0/28320

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	10316	0	10452	135	0
2	B	2575	0	2619	35	0
3	C	7570	0	7368	119	0
4	D	28	0	25	2	0
4	E	28	0	25	1	0
4	G	28	0	25	1	0
4	H	28	0	25	3	0
5	F	56	0	49	4	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	140	0	230	10	0
8	A	76	0	103	1	0
9	A	64	0	66	5	0
10	C	42	0	39	2	0
All	All	20953	0	21026	295	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 7.

All (295) 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:113:PRO:HG3	1:A:630:ASN:HD21	1.38	0.87
3:C:895:ASN:HB3	4:H:1:NAG:H2	1.67	0.76
3:C:1001:ARG:HG2	3:C:1019:GLU:HB2	1.66	0.75
1:A:1401:ILE:HD11	7:A:2402:CLR:H181	1.70	0.74
1:A:89:PRO:HB2	1:A:90:PRO:HD3	1.69	0.72
3:C:468:ASN:OD1	5:F:1:NAG:N2	2.24	0.69
3:C:884:ARG:NH1	3:C:1029:ARG:O	2.26	0.68
1:A:1412:PHE:O	1:A:1416:ASN:ND2	2.28	0.66
9:A:2409:PT5:H36	9:A:2409:PT5:H69	1.77	0.65
1:A:1190:ASP:OD1	1:A:1264:ARG:NH2	2.27	0.65
1:A:485:LEU:HD13	1:A:518:LEU:HD21	1.77	0.65
3:C:859:LEU:HD21	3:C:867:TYR:HB3	1.79	0.65
3:C:734:VAL:HG23	3:C:812:VAL:HG12	1.79	0.64
3:C:979:THR:HG23	3:C:1033:GLN:HG2	1.80	0.63
3:C:716:VAL:HA	3:C:720:TRP:HB2	1.80	0.63
1:A:323:GLY:O	1:A:327:ASN:ND2	2.33	0.62
2:B:323:ASP:O	2:B:327:GLN:NE2	2.32	0.62
3:C:568:ASN:HB3	3:C:571:LYS:HG2	1.81	0.62
1:A:1673:LEU:HD23	1:A:1699:ALA:HB3	1.79	0.62
3:C:357:ILE:HG22	3:C:383:ARG:HB2	1.81	0.62
1:A:1143:ARG:NH2	1:A:1207:ASP:O	2.33	0.62
3:C:570:ILE:HD13	3:C:586:LYS:HE3	1.82	0.62
1:A:1736:LEU:HD13	1:A:1739:HIS:HB3	1.81	0.62
1:A:390:ALA:HB2	2:B:199:ALA:HB2	1.81	0.61
3:C:59:ASP:HA	3:C:62:GLU:HG2	1.83	0.61
3:C:28:PRO:HB2	3:C:33:ILE:HD11	1.82	0.61
1:A:234:MET:HG2	8:A:2406:3PE:H3F2	1.82	0.60
1:A:139:ALA:O	1:A:143:ILE:HG13	2.02	0.60
2:B:128:ARG:NH1	2:B:160:GLN:OE1	2.35	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:MET:SD	1:A:472:MET:N	2.74	0.60
1:A:392:GLU:HG3	1:A:471:HIS:HD2	1.66	0.59
3:C:442:LYS:NZ	3:C:465:PRO:O	2.34	0.59
2:B:214:ILE:HA	2:B:268:VAL:HG22	1.83	0.59
3:C:591:LEU:HD11	3:C:895:ASN:HD21	1.66	0.59
3:C:860:LEU:HD12	3:C:1013:LEU:HD21	1.84	0.58
1:A:394:MET:HB3	2:B:198:LYS:HE3	1.84	0.58
3:C:313:ARG:HD2	3:C:534:VAL:HG23	1.84	0.58
3:C:708:ASP:HA	3:C:711:PHE:HB2	1.86	0.58
3:C:157:ARG:NH2	3:C:222:PRO:O	2.36	0.58
5:F:4:NAG:H3	5:F:4:NAG:H83	1.86	0.58
2:B:291:PHE:HB3	2:B:336:ILE:HD12	1.86	0.58
3:C:717:GLN:O	3:C:721:SER:OG	2.21	0.58
1:A:1617:LEU:HD13	1:A:1713:LEU:HD12	1.86	0.57
3:C:240:ARG:NH2	3:C:278:GLU:O	2.37	0.57
3:C:666:TYR:O	3:C:698:ASN:ND2	2.37	0.57
1:A:85:LEU:HG	1:A:88:TRP:NE1	2.19	0.57
1:A:1658:ARG:HH11	1:A:1668:ILE:HD11	1.68	0.57
1:A:654:LEU:HD22	1:A:690:GLY:HA3	1.87	0.56
3:C:646:GLU:HA	3:C:649:LYS:HD3	1.86	0.56
1:A:1748:TRP:HB2	1:A:1805:PHE:HE2	1.70	0.56
2:B:179:PRO:HG3	2:B:257:ILE:HD11	1.86	0.56
4:D:2:NAG:H3	4:D:2:NAG:H83	1.87	0.56
3:C:849:ASP:OD1	3:C:849:ASP:N	2.39	0.56
1:A:589:LEU:HG	9:A:2409:PT5:H28	1.87	0.56
1:A:520:LEU:HD11	1:A:552:ILE:HD11	1.88	0.56
3:C:109:ALA:HA	3:C:470:THR:HG22	1.88	0.56
1:A:88:TRP:HB3	1:A:91:PHE:HB3	1.88	0.55
3:C:729:VAL:HG22	3:C:814:ILE:HD12	1.88	0.55
1:A:1743:GLU:O	1:A:1746:ARG:HG3	2.06	0.55
1:A:1350:ARG:NH1	1:A:1356:ASP:OD2	2.40	0.54
3:C:817:ASP:N	3:C:817:ASP:OD1	2.35	0.54
1:A:508:LEU:O	1:A:512:GLU:HG2	2.07	0.54
3:C:786:GLY:HA2	3:C:789:GLU:HG2	1.88	0.54
2:B:173:VAL:O	2:B:284:SER:OG	2.26	0.54
3:C:902:SER:OG	3:C:974:CYS:O	2.25	0.54
3:C:534:VAL:HA	3:C:975:ILE:HD11	1.90	0.54
3:C:747:GLU:CD	3:C:747:GLU:H	2.11	0.54
1:A:376:ILE:HD11	2:B:298:LYS:HD2	1.89	0.54
1:A:358:ARG:NH2	1:A:711:GLU:OE1	2.38	0.54
2:B:73:VAL:O	2:B:81:GLN:NE2	2.40	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:667:CYS:HB3	3:C:697:CYS:HA	1.90	0.53
1:A:284:GLY:HA3	1:A:288:GLY:HA2	1.90	0.53
1:A:1397:MET:HB3	7:A:2402:CLR:H6	1.90	0.53
3:C:720:TRP:HB3	3:C:744:TYR:HD2	1.74	0.53
1:A:211:LEU:HB2	1:A:609:LEU:HD21	1.91	0.53
2:B:173:VAL:HB	2:B:226:ARG:HH22	1.74	0.53
1:A:102:ASN:OD1	1:A:196:ARG:NH1	2.42	0.52
1:A:1424:ILE:HG13	1:A:1425:THR:HG23	1.91	0.52
1:A:122:ARG:HH12	3:C:330:ILE:HG21	1.74	0.52
3:C:280:LEU:HA	3:C:283:LEU:HD12	1.91	0.52
2:B:198:LYS:NZ	2:B:202:ASP:OD2	2.42	0.52
1:A:85:LEU:HG	1:A:88:TRP:CD1	2.44	0.52
2:B:344:ASP:N	2:B:344:ASP:OD1	2.42	0.52
2:B:212:ILE:HG13	2:B:266:LEU:HD22	1.90	0.52
3:C:661:ILE:O	3:C:676:ASN:ND2	2.29	0.52
1:A:1157:MET:O	1:A:1161:LEU:HD22	2.10	0.52
3:C:644:TYR:CE1	3:C:710:GLY:HA3	2.45	0.52
1:A:1374:TRP:CD1	1:A:1375:PRO:HD3	2.45	0.52
1:A:359:GLU:OE2	1:A:786:ARG:NH1	2.43	0.51
3:C:1027:ASP:N	3:C:1027:ASP:OD1	2.42	0.51
2:B:50:GLN:OE1	2:B:54:ARG:NH1	2.44	0.51
2:B:277:PRO:HB3	2:B:289:ILE:HD13	1.92	0.51
1:A:1591:TYR:O	1:A:1595:ILE:HG13	2.11	0.51
3:C:851:VAL:HG12	3:C:862:ALA:HA	1.93	0.51
3:C:782:LYS:NZ	10:C:1202:NAG:O7	2.41	0.51
3:C:786:GLY:O	3:C:790:SER:OG	2.24	0.51
1:A:1528:LYS:HD2	1:A:1532:PHE:HE2	1.76	0.50
3:C:726:ILE:HB	3:C:729:VAL:HB	1.93	0.50
1:A:591:ASN:ND2	1:A:713:THR:OG1	2.39	0.50
1:A:1455:PRO:HG3	1:A:1748:TRP:HE1	1.76	0.50
2:B:216:ARG:HG3	2:B:270:ASP:HB2	1.94	0.50
3:C:33:ILE:HG21	3:C:1004:HIS:HD2	1.75	0.49
3:C:568:ASN:OD1	3:C:569:ASP:N	2.45	0.49
1:A:174:ALA:HA	1:A:189:LEU:HD22	1.94	0.49
3:C:284:SER:OG	3:C:285:ASP:N	2.46	0.49
3:C:466:VAL:HG12	3:C:485:LEU:HD12	1.93	0.49
3:C:613:ASN:OD1	4:G:1:NAG:N2	2.45	0.49
3:C:798:VAL:HG23	3:C:809:PRO:HD2	1.92	0.49
3:C:1067:ASP:OD2	3:C:1069:THR:OG1	2.26	0.49
3:C:1061:ASP:OD1	3:C:1061:ASP:N	2.46	0.49
1:A:287:ASP:OD2	1:A:668:ARG:NH1	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:PRO:HB3	2:B:322:TYR:HE2	1.78	0.49
3:C:61:TYR:O	3:C:68:TYR:OH	2.27	0.49
1:A:1791:VAL:HG22	1:A:1792:LEU:H	1.78	0.49
4:E:2:NAG:O7	4:E:2:NAG:O4	2.20	0.49
3:C:861:MET:HE3	3:C:861:MET:HA	1.94	0.48
1:A:228:LEU:HD13	1:A:342:VAL:HG21	1.93	0.48
2:B:304:ILE:HG21	2:B:315:LEU:HD13	1.94	0.48
3:C:79:VAL:HG12	3:C:610:THR:HG22	1.95	0.48
1:A:253:MET:HB2	1:A:278:GLU:H	1.77	0.48
1:A:226:LEU:HB3	1:A:1593:ILE:HD11	1.94	0.48
1:A:1508:LEU:HG	1:A:1512:TYR:CE1	2.48	0.48
3:C:802:ILE:HG22	3:C:803:GLN:HG2	1.95	0.48
1:A:1165:ALA:HB1	7:A:2405:CLR:H273	1.94	0.48
2:B:181:VAL:HG12	2:B:269:LEU:HD22	1.95	0.48
3:C:516:ASP:OD1	3:C:517:PRO:HD2	2.14	0.48
3:C:1039:ASP:OD1	3:C:1039:ASP:N	2.46	0.48
1:A:367:PHE:CZ	1:A:711:GLU:HB3	2.49	0.48
1:A:590:ARG:HG3	9:A:2409:PT5:H2	1.96	0.47
1:A:680:ALA:O	1:A:684:ILE:HG12	2.14	0.47
3:C:363:ASP:OD1	3:C:364:GLY:N	2.46	0.47
1:A:1827:ASP:OD1	1:A:1827:ASP:N	2.45	0.47
1:A:389:LYS:HA	1:A:389:LYS:HD2	1.63	0.47
3:C:594:SER:OG	3:C:596:ASP:O	2.32	0.47
1:A:1488:ILE:O	1:A:1492:THR:HG23	2.14	0.47
1:A:1492:THR:HG21	1:A:1586:LEU:HD23	1.97	0.47
1:A:1736:LEU:HD12	1:A:1740:HIS:HB2	1.96	0.47
3:C:128:LYS:HB3	3:C:223:TRP:HB3	1.97	0.47
3:C:149:PHE:CE1	3:C:222:PRO:HD3	2.50	0.47
1:A:1493:VAL:HG22	7:A:2407:CLR:H271	1.96	0.47
1:A:1536:ASN:O	1:A:1536:ASN:ND2	2.44	0.47
3:C:174:GLU:HA	3:C:179:VAL:HG11	1.96	0.47
3:C:875:PHE:HB3	3:C:883:MET:SD	2.54	0.47
1:A:1449:PHE:CD2	1:A:1741:LEU:HD13	2.49	0.47
2:B:179:PRO:HB3	2:B:267:VAL:HG13	1.97	0.47
3:C:666:TYR:HB3	3:C:702:ILE:HD11	1.96	0.47
7:A:2407:CLR:H211	7:A:2407:CLR:H232	1.80	0.46
1:A:473:VAL:HG23	1:A:474:LYS:HD3	1.97	0.46
1:A:1497:MET:HG2	1:A:1506:TYR:OH	2.15	0.46
1:A:1553:SER:O	1:A:1557:ILE:HG22	2.15	0.46
1:A:1839:THR:HB	1:A:1842:ILE:HG12	1.97	0.46
3:C:827:LYS:HB2	3:C:827:LYS:HE2	1.75	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:ASN:ND2	3:C:328:LYS:O	2.32	0.46
1:A:141:ILE:O	1:A:145:ALA:HB3	2.16	0.46
3:C:289:VAL:HG12	3:C:310:ALA:HB2	1.98	0.46
3:C:468:ASN:OD1	3:C:485:LEU:HD21	2.16	0.46
3:C:596:ASP:OD1	3:C:596:ASP:N	2.48	0.46
1:A:1795:MET:HG2	1:A:1797:VAL:HG23	1.97	0.46
1:A:128:GLU:OE2	1:A:196:ARG:NH2	2.44	0.46
1:A:1457:THR:HG23	1:A:1459:TYR:H	1.80	0.46
3:C:75:ALA:O	3:C:79:VAL:HG23	2.16	0.46
3:C:351:ARG:HH22	3:C:356:LYS:HD3	1.81	0.46
1:A:1607:LEU:HD12	1:A:1607:LEU:O	2.15	0.45
3:C:205:TRP:NE1	3:C:456:LEU:HD22	2.31	0.45
1:A:1160:LEU:HD21	1:A:1271:ARG:HB3	1.98	0.45
1:A:716:GLU:O	1:A:720:GLU:HG2	2.16	0.45
3:C:254:MET:O	3:C:289:VAL:HA	2.17	0.45
3:C:855:ASP:HB2	3:C:1012:ASN:HB2	1.99	0.45
1:A:135:PHE:O	1:A:138:GLU:HG3	2.16	0.45
2:B:257:ILE:HD13	2:B:285:LEU:HD13	1.99	0.45
1:A:636:PRO:O	1:A:639:ASN:ND2	2.43	0.45
1:A:112:LEU:HD13	3:C:263:SER:HB3	1.98	0.45
1:A:164:ASP:OD1	1:A:199:LYS:HG2	2.16	0.45
1:A:1409:VAL:O	1:A:1413:PHE:HB3	2.17	0.45
1:A:471:HIS:O	1:A:471:HIS:ND1	2.49	0.45
1:A:1731:ARG:HD3	1:A:1731:ARG:HA	1.88	0.45
7:A:2404:CLR:H162	7:A:2404:CLR:H221	1.64	0.45
2:B:140:ASN:OD1	2:B:141:PRO:HD3	2.17	0.45
5:F:3:NAG:H4	5:F:4:NAG:H2	1.66	0.45
1:A:135:PHE:HE2	1:A:196:ARG:HH11	1.65	0.44
3:C:273:ARG:HD2	3:C:323:ASN:HA	1.99	0.44
3:C:712:THR:HG23	3:C:734:VAL:HG11	1.98	0.44
1:A:1775:LEU:HD23	1:A:1775:LEU:HA	1.86	0.44
2:B:121:PRO:HA	2:B:124:LEU:HB2	1.98	0.44
3:C:596:ASP:OD1	3:C:762:SER:OG	2.35	0.44
1:A:1210:LEU:HD23	1:A:1210:LEU:HA	1.81	0.44
1:A:275:ALA:O	1:A:277:TYR:N	2.45	0.44
1:A:1777:LEU:HD23	1:A:1777:LEU:HA	1.83	0.44
2:B:208:PHE:HA	2:B:211:ARG:NH2	2.33	0.44
2:B:296:SER:HB2	2:B:298:LYS:HE2	1.99	0.44
1:A:633:ASP:OD1	1:A:633:ASP:N	2.39	0.44
3:C:658:TYR:HD2	3:C:746:LYS:HG3	1.83	0.44
1:A:1780:ARG:HA	1:A:1780:ARG:HD3	1.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:VAL:HB	2:B:268:VAL:HA	2.00	0.43
2:B:134:LYS:HD3	2:B:134:LYS:HA	1.80	0.43
1:A:312:THR:HG21	1:A:1658:ARG:HG3	2.00	0.43
1:A:1234:LEU:HA	1:A:1237:PHE:CE1	2.53	0.43
3:C:241:ARG:HA	3:C:241:ARG:HD2	1.86	0.43
1:A:142:LYS:O	1:A:146:LEU:HB3	2.18	0.43
1:A:263:ASP:O	1:A:265:PRO:HD3	2.19	0.43
3:C:42:GLU:O	3:C:46:THR:OG1	2.25	0.43
3:C:895:ASN:CB	4:H:1:NAG:H2	2.43	0.43
1:A:1285:SER:O	1:A:1289:VAL:HG23	2.18	0.43
7:A:2402:CLR:H211	7:A:2402:CLR:H232	1.85	0.43
2:B:153:PRO:HA	2:B:154:PRO:HD3	1.92	0.43
3:C:253:ASP:OD2	3:C:351:ARG:NH2	2.50	0.43
1:A:85:LEU:HG	1:A:88:TRP:HE1	1.82	0.43
3:C:849:ASP:HB3	3:C:864:HIS:NE2	2.34	0.43
1:A:89:PRO:CB	1:A:90:PRO:HD3	2.44	0.43
1:A:638:ALA:HB1	1:A:649:THR:HG23	2.00	0.43
7:A:2402:CLR:H221	7:A:2402:CLR:H162	1.40	0.43
3:C:862:ALA:HB1	3:C:867:TYR:HB2	2.01	0.43
3:C:114:ARG:NH2	3:C:120:ASN:HB2	2.33	0.43
1:A:540:PHE:CE1	9:A:2409:PT5:H18	2.54	0.42
1:A:1510:LEU:HD23	1:A:1510:LEU:HA	1.90	0.42
3:C:580:ASP:N	3:C:580:ASP:OD1	2.51	0.42
1:A:1673:LEU:O	1:A:1676:LYS:NZ	2.30	0.42
1:A:1771:MET:HG2	1:A:1772:SER:N	2.35	0.42
3:C:159:ILE:HG22	3:C:221:SER:OG	2.19	0.42
3:C:432:ARG:HB2	3:C:433:PRO:HD3	2.02	0.42
1:A:190:ARG:O	1:A:193:ARG:HG2	2.20	0.42
3:C:271:LEU:O	3:C:275:SER:OG	2.25	0.42
1:A:89:PRO:HB2	1:A:90:PRO:CD	2.46	0.42
1:A:164:ASP:O	1:A:168:VAL:HG23	2.20	0.42
1:A:1522:SER:HA	1:A:1550:VAL:HG21	2.01	0.42
3:C:73:ASN:N	3:C:628:PHE:O	2.52	0.42
3:C:506:LEU:HD12	3:C:623:LEU:HD13	2.02	0.42
3:C:735:VAL:HB	3:C:811:VAL:HG12	2.02	0.42
2:B:125:GLU:HA	2:B:128:ARG:HG2	2.01	0.42
1:A:1337:GLU:HG3	1:A:1338:LYS:HG3	2.02	0.42
2:B:223:LEU:HA	2:B:225:LYS:HE2	2.01	0.42
3:C:849:ASP:HA	3:C:863:ASN:HD22	1.84	0.42
3:C:377:ASN:OD1	3:C:377:ASN:O	2.38	0.42
1:A:593:VAL:HG21	9:A:2409:PT5:H21	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:LEU:HA	1:A:1228:VAL:HG12	2.01	0.41
1:A:295:ILE:HG12	1:A:1496:MET:HB2	2.00	0.41
5:F:1:NAG:H62	5:F:2:NAG:H82	2.02	0.41
1:A:1222:TRP:CD1	1:A:1270:LYS:HB2	2.55	0.41
1:A:1742:ASP:OD1	1:A:1743:GLU:N	2.51	0.41
3:C:57:LEU:HD22	3:C:715:LEU:HD22	2.01	0.41
3:C:147:PRO:HB3	3:C:163:HIS:NE2	2.35	0.41
1:A:1522:SER:O	1:A:1526:VAL:HG13	2.21	0.41
7:A:2402:CLR:H183	7:A:2402:CLR:H20	1.97	0.41
3:C:720:TRP:HB3	3:C:744:TYR:CD2	2.54	0.41
3:C:781:ASN:HD22	10:C:1202:NAG:H62	1.84	0.41
1:A:214:ILE:HD11	1:A:606:LEU:HD23	2.01	0.41
1:A:1325:THR:HG22	1:A:1328:GLU:HG3	2.03	0.41
1:A:1748:TRP:HB2	1:A:1805:PHE:CE2	2.52	0.41
3:C:37:VAL:HG21	3:C:1006:GLU:HB3	2.03	0.41
3:C:648:LEU:HB3	3:C:680:LEU:HD11	2.02	0.41
3:C:854:ASP:HA	3:C:1013:LEU:HD23	2.02	0.41
1:A:355:ALA:HB2	1:A:778:TRP:CZ3	2.56	0.41
1:A:1340:LYS:HA	1:A:1340:LYS:HD3	1.85	0.41
1:A:1462:GLN:O	1:A:1464:ARG:NH2	2.53	0.41
3:C:526:ASN:ND2	3:C:564:ALA:O	2.35	0.41
2:B:60:VAL:HG12	2:B:96:LYS:HG2	2.02	0.41
3:C:120:ASN:ND2	4:D:2:NAG:O7	2.54	0.41
3:C:777:ALA:HA	3:C:860:LEU:HD21	2.01	0.41
1:A:154:SER:OG	1:A:155:TYR:N	2.53	0.41
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.91	0.41
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.90	0.41
1:A:1374:TRP:CG	1:A:1375:PRO:HD3	2.55	0.41
1:A:1460:MET:O	1:A:1462:GLN:NE2	2.53	0.41
1:A:1658:ARG:NH1	1:A:1668:ILE:HD11	2.35	0.41
2:B:144:LEU:HD12	2:B:144:LEU:HA	1.91	0.41
3:C:29:SER:HB3	3:C:32:THR:HG23	2.03	0.41
3:C:296:SER:HA	3:C:332:ASP:HB2	2.03	0.41
3:C:660:PHE:O	3:C:740:ILE:HG22	2.21	0.41
3:C:886:LEU:HD23	3:C:889:ILE:HD11	2.02	0.41
3:C:895:ASN:HB3	4:H:1:NAG:C2	2.42	0.41
1:A:1307:ALA:HB2	1:A:1402:PHE:CZ	2.56	0.41
3:C:67:LEU:HD12	3:C:67:LEU:H	1.87	0.40
3:C:1070:ASP:OD1	3:C:1070:ASP:N	2.39	0.40
3:C:61:TYR:HB2	3:C:800:ILE:HD12	2.04	0.40
3:C:351:ARG:HE	3:C:351:ARG:HB3	1.62	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:694:ASN:HB3	3:C:697:CYS:O	2.21	0.40
3:C:849:ASP:HB3	3:C:864:HIS:CD2	2.56	0.40
1:A:377:GLU:OE1	2:B:302:ARG:NH2	2.54	0.40
1:A:1312:LYS:HB3	1:A:1312:LYS:HE2	1.75	0.40
1:A:1337:GLU:C	1:A:1338:LYS:HG3	2.42	0.40
1:A:1458:ARG:HH22	1:A:1472:TRP:HZ2	1.69	0.40
1:A:1665:TRP:HA	1:A:1668:ILE:HD12	2.02	0.40
3:C:29:SER:O	3:C:33:ILE:HG12	2.21	0.40
3:C:103:GLU:HG2	3:C:192:VAL:HG21	2.04	0.40
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.93	0.40
1:A:246:LYS:HB3	1:A:322:LEU:HD21	2.04	0.40
1:A:1197:PHE:HA	1:A:1200:GLU:OE1	2.21	0.40
1:A:1653:LEU:HD23	1:A:1653:LEU:HA	1.94	0.40
2:B:123:ARG:HE	2:B:127:ILE:HG13	1.86	0.40
1:A:253:MET:HB2	1:A:278:GLU:N	2.37	0.40
1:A:1562:SER:O	1:A:1566:ASN:ND2	2.51	0.40
1:A:1839:THR:O	1:A:1842:ILE:HG12	2.21	0.40
7:A:2404:CLR:H213	7:A:2404:CLR:H231	1.85	0.40
3:C:54:VAL:O	3:C:58:VAL:HG23	2.22	0.40
3:C:582:GLU:O	3:C:609:TRP:NE1	2.53	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	1258/2313 (54%)	1203 (96%)	54 (4%)	1 (0%)	48 79
2	B	322/484 (66%)	311 (97%)	10 (3%)	1 (0%)	37 68
3	C	936/1103 (85%)	885 (95%)	51 (5%)	0	100 100
All	All	2516/3900 (64%)	2399 (95%)	115 (5%)	2 (0%)	50 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
2	B	287	PRO

### 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	1123/2023 (56%)	1102 (98%)	21 (2%)	52	75
2	B	287/426 (67%)	285 (99%)	2 (1%)	81	90
3	C	837/971 (86%)	825 (99%)	12 (1%)	62	81
All	All	2247/3420 (66%)	2212 (98%)	35 (2%)	58	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	186	LEU
1	A	196	ARG
1	A	253	MET
1	A	373	GLN
1	A	394	MET
1	A	541	ASN
1	A	789	MET
1	A	1153	ARG
1	A	1237	PHE
1	A	1311	PHE
1	A	1324	ASP
1	A	1338	LYS
1	A	1491	ASN
1	A	1535	LEU
1	A	1536	ASN
1	A	1540	ASP
1	A	1561	ASP
1	A	1604	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1626	MET
1	A	1810	MET
2	B	319	MET
2	B	331	GLU
3	C	43	ASP
3	C	152	ASP
3	C	476	LYS
3	C	590	THR
3	C	591	LEU
3	C	595	GLN
3	C	744	TYR
3	C	817	ASP
3	C	865	ASP
3	C	974	CYS
3	C	999	CYS
3	C	1029	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	4,3	14,14,15	0.35	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.44	0	17,19,21	1.34	2 (11%)
4	NAG	E	1	4,3	14,14,15	0.55	0	17,19,21	0.45	0
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	0.84	0
5	NAG	F	1	5,3	14,14,15	0.38	0	17,19,21	0.67	0
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	F	3	5	14,14,15	1.05	1 (7%)	17,19,21	1.25	1 (5%)
5	NAG	F	4	5	14,14,15	0.62	1 (7%)	17,19,21	1.33	2 (11%)
4	NAG	G	1	4,3	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	H	1	4,3	14,14,15	0.81	1 (7%)	17,19,21	0.64	0
4	NAG	H	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.22	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	NAG	E	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
5	NAG	F	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	3	5	-	2/6/23/26	0/1/1/1
5	NAG	F	4	5	-	6/6/23/26	0/1/1/1
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	NAG	O5-C1	3.64	1.49	1.43
4	H	2	NAG	O5-C1	3.27	1.49	1.43
4	H	1	NAG	C1-C2	2.52	1.55	1.52
5	F	4	NAG	C1-C2	2.07	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	NAG	C1-O5-C5	4.94	118.81	112.19
4	H	2	NAG	C1-O5-C5	4.60	118.35	112.19
4	D	2	NAG	C2-N2-C7	4.55	129.00	122.90
5	F	4	NAG	C2-N2-C7	4.55	128.99	122.90
5	F	4	NAG	C1-C2-N2	2.17	113.85	110.43
4	D	2	NAG	C1-C2-N2	2.10	113.74	110.43

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

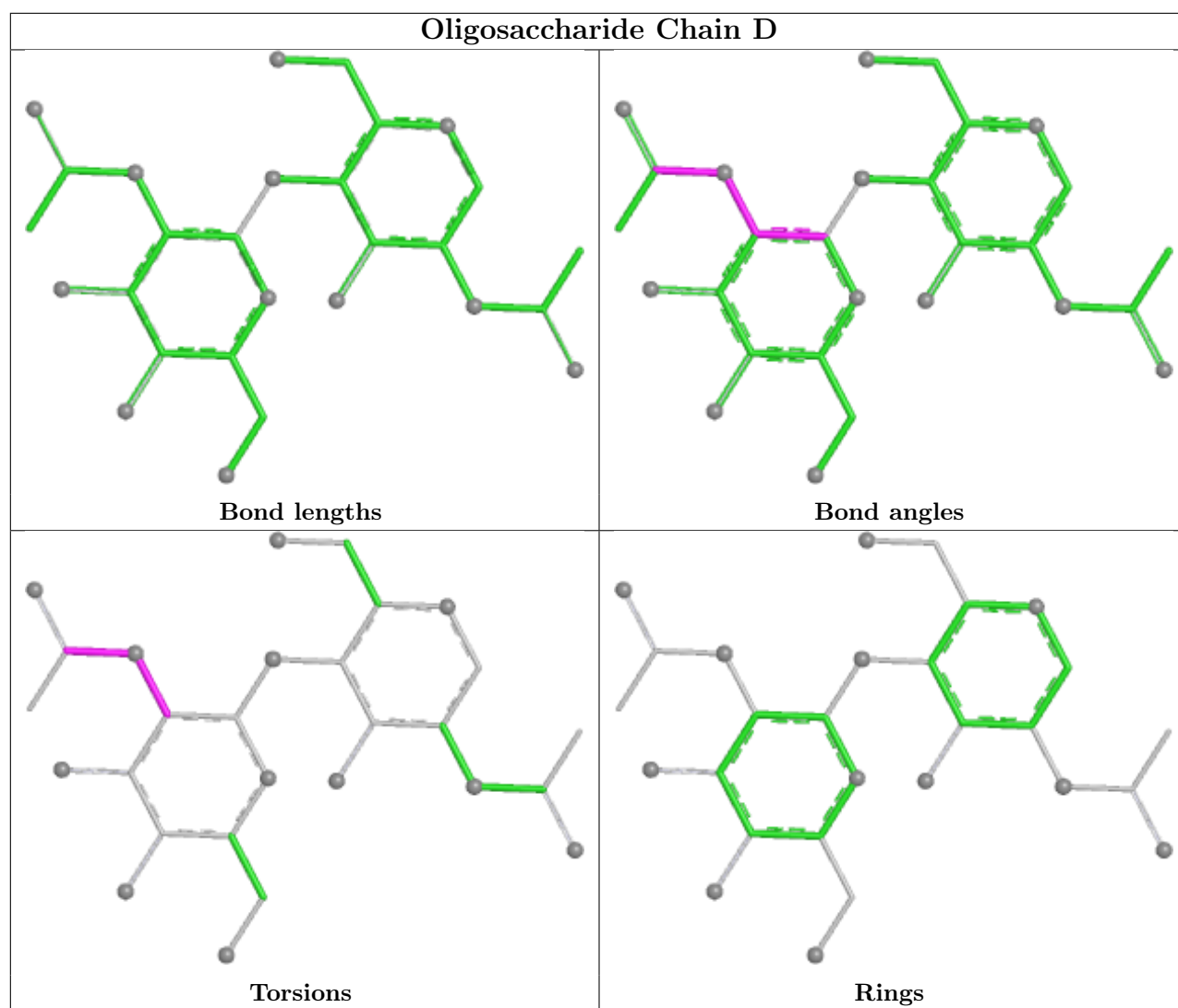
Mol	Chain	Res	Type	Atoms
5	F	4	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6

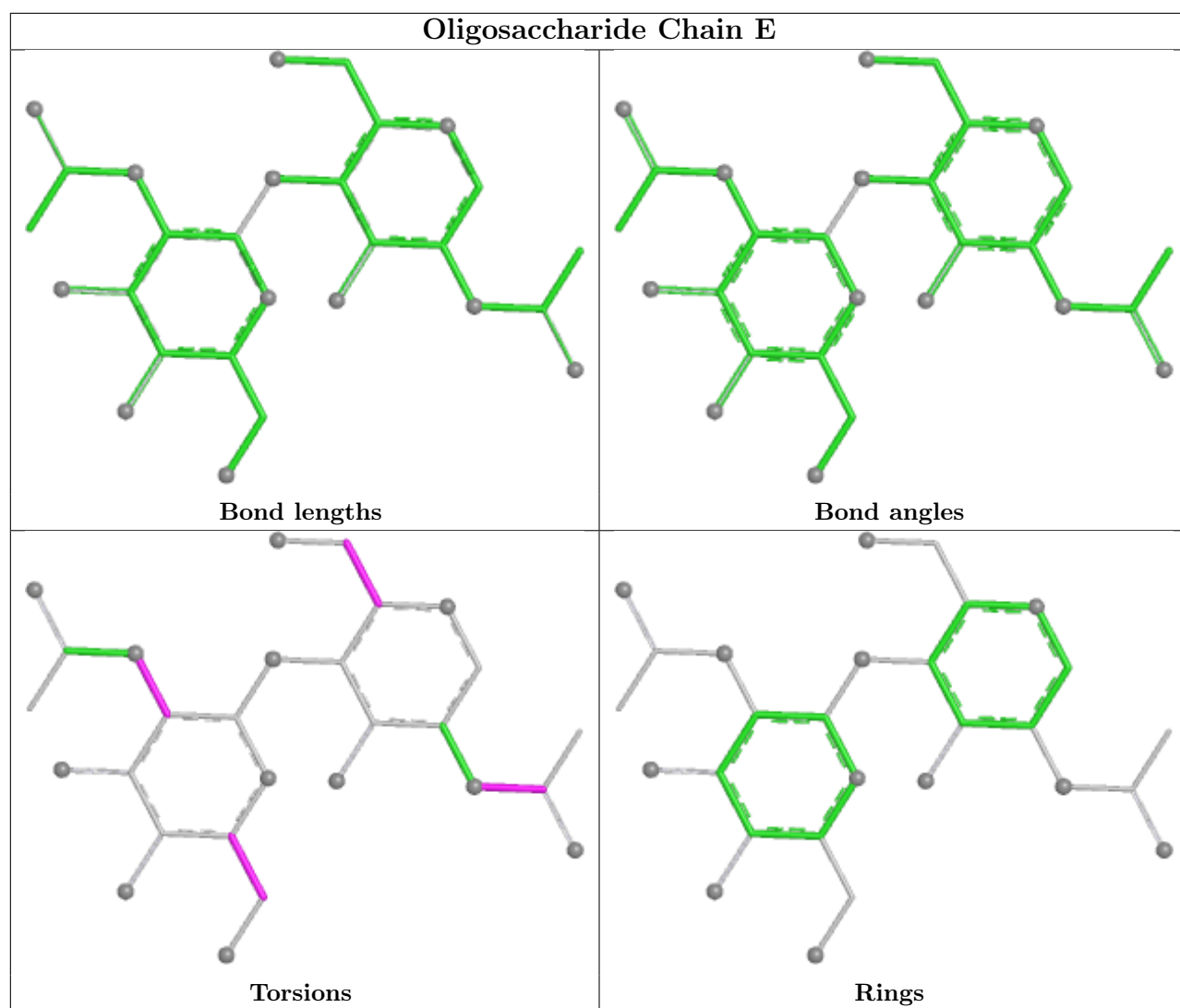
There are no ring outliers.

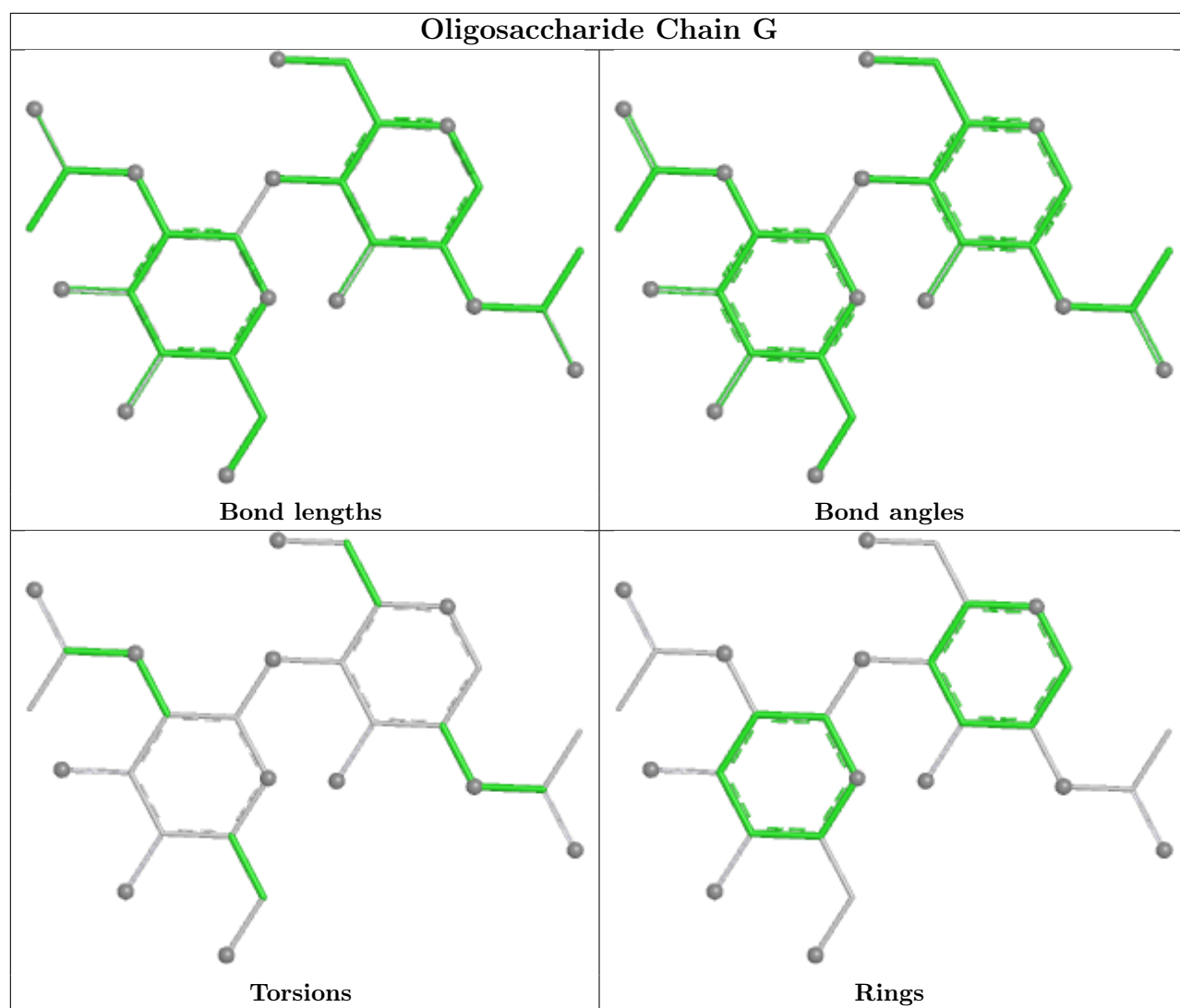
8 monomers are involved in 11 short contacts:

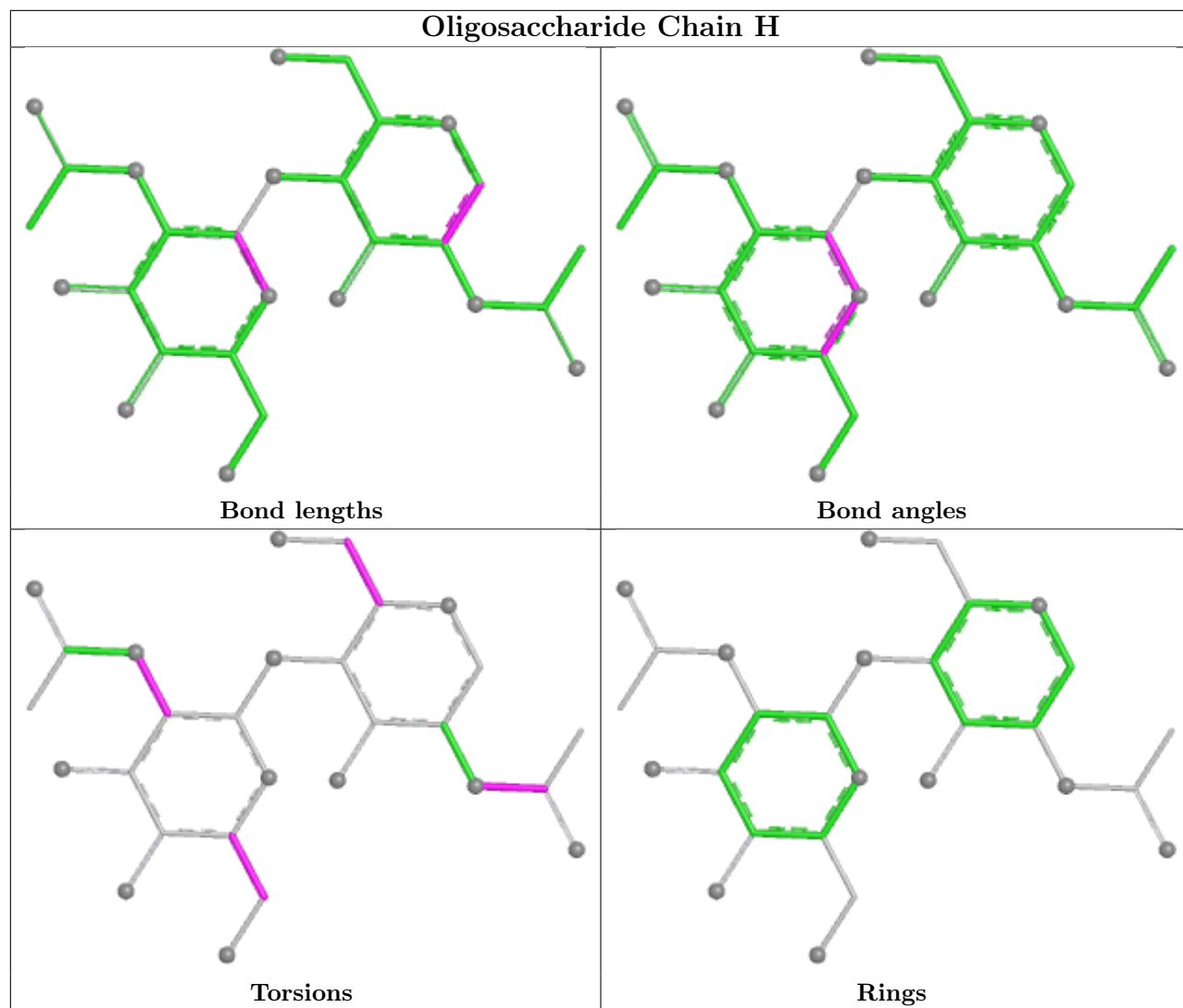
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	2	0
4	E	2	NAG	1	0
5	F	4	NAG	2	0
5	F	3	NAG	1	0
5	F	2	NAG	1	0
4	G	1	NAG	1	0
4	D	2	NAG	2	0
4	H	1	NAG	3	0

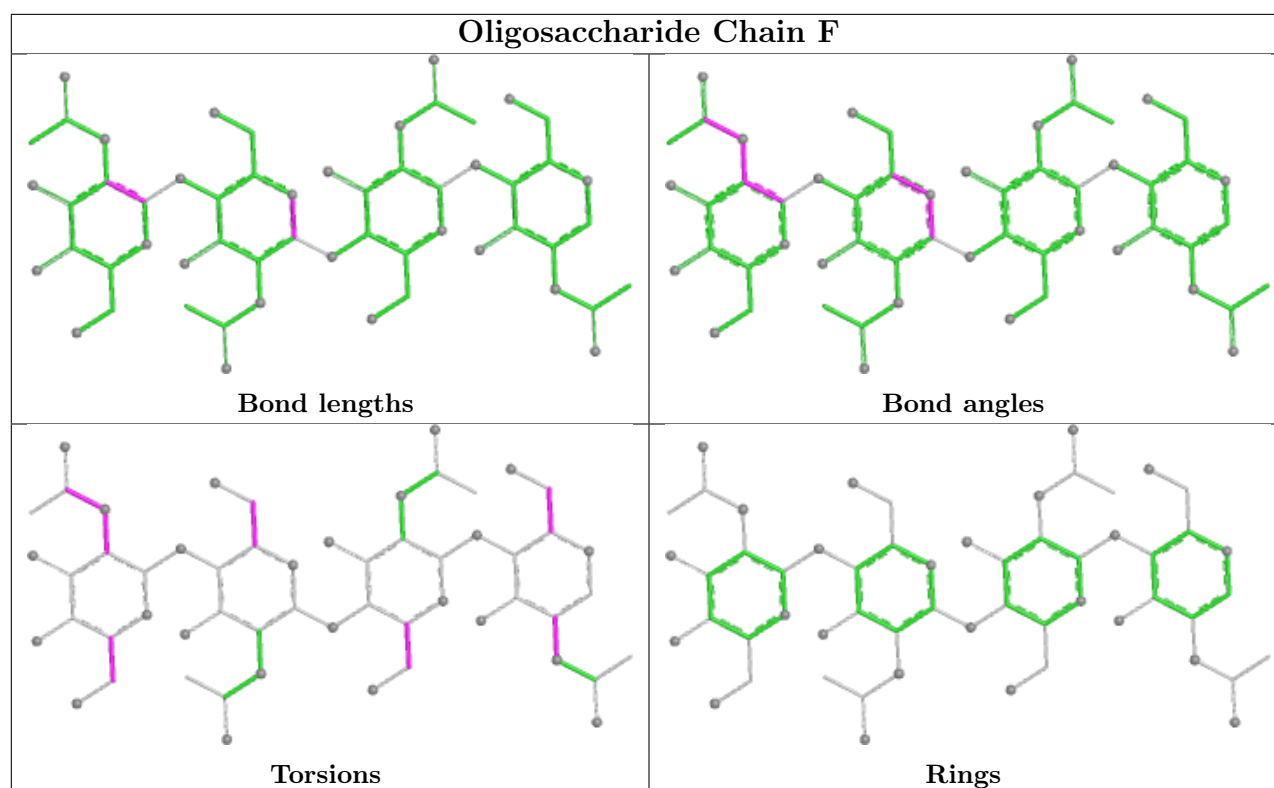
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	CLR	A	2407	-	31,31,31	0.37	0	48,48,48	0.68	1 (2%)
10	NAG	C	1201	3	14,14,15	0.45	0	17,19,21	0.51	0
10	NAG	C	1202	3	14,14,15	0.80	1 (7%)	17,19,21	0.98	1 (5%)
7	CLR	A	2403	-	31,31,31	0.38	0	48,48,48	0.56	0
10	NAG	C	1203	-	14,14,15	0.18	0	17,19,21	0.48	0
7	CLR	A	2405	-	31,31,31	0.37	0	48,48,48	0.55	0
8	3PE	A	2406	-	40,40,50	0.56	0	43,45,55	0.65	2 (4%)
9	PT5	A	2409	-	64,64,69	1.38	7 (10%)	79,82,87	1.20	6 (7%)
7	CLR	A	2402	-	31,31,31	0.39	0	48,48,48	0.78	0
8	3PE	A	2408	-	34,34,50	0.61	0	37,39,55	0.63	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLR	A	2404	-	31,31,31	0.41	0	48,48,48	0.67	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	CLR	A	2407	-	-	7/10/68/68	0/4/4/4
10	NAG	C	1201	3	-	2/6/23/26	0/1/1/1
10	NAG	C	1202	3	-	2/6/23/26	0/1/1/1
7	CLR	A	2403	-	-	1/10/68/68	0/4/4/4
10	NAG	C	1203	-	-	4/6/23/26	0/1/1/1
7	CLR	A	2405	-	-	8/10/68/68	0/4/4/4
8	3PE	A	2406	-	-	16/44/44/54	-
9	PT5	A	2409	-	-	33/61/85/90	0/1/1/1
7	CLR	A	2402	-	-	7/10/68/68	0/4/4/4
8	3PE	A	2408	-	-	10/38/38/54	-
7	CLR	A	2404	-	-	6/10/68/68	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2409	PT5	P4-O4	4.02	1.66	1.59
9	A	2409	PT5	P5-O5	3.78	1.66	1.59
9	A	2409	PT5	O18-C11	3.55	1.43	1.33
9	A	2409	PT5	P1-O1	2.95	1.68	1.59
9	A	2409	PT5	C31-C11	2.68	1.58	1.50
9	A	2409	PT5	O16-C8	-2.67	1.40	1.46
9	A	2409	PT5	O16-C10	2.66	1.41	1.34
10	C	1202	NAG	O5-C1	2.53	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2409	PT5	O16-C10-C12	3.92	119.97	111.48
10	C	1202	NAG	C1-O5-C5	3.82	117.30	112.19
9	A	2409	PT5	C23-C22-C21	3.50	153.07	123.57
9	A	2409	PT5	C17-C16-C15	3.44	152.59	123.57
9	A	2409	PT5	C20-C19-C18	3.36	151.89	123.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2409	PT5	O18-C11-C31	2.67	119.97	111.83
8	A	2408	3PE	O12-P-O14	2.44	123.80	112.44
8	A	2406	3PE	O12-P-O14	2.42	123.70	112.44
8	A	2406	3PE	C2-O21-C21	2.36	123.44	117.80
9	A	2409	PT5	C5-C6-C1	2.34	113.85	109.11
7	A	2407	CLR	C16-C17-C13	-2.05	101.43	103.84

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2406	3PE	C11-O13-P-O12
8	A	2406	3PE	C11-O13-P-O14
8	A	2408	3PE	C1-O11-P-O14
8	A	2408	3PE	O13-C11-C12-N
9	A	2409	PT5	C3-C4-O4-P4
9	A	2409	PT5	C5-C4-O4-P4
9	A	2409	PT5	C18-C19-C20-C21
9	A	2409	PT5	O19-C11-O18-C9
9	A	2409	PT5	C31-C11-O18-C9
7	A	2402	CLR	C16-C17-C20-C21
7	A	2402	CLR	C13-C17-C20-C21
7	A	2402	CLR	C16-C17-C20-C22
7	A	2402	CLR	C21-C20-C22-C23
7	A	2407	CLR	C21-C20-C22-C23
7	A	2402	CLR	C13-C17-C20-C22
7	A	2407	CLR	C13-C17-C20-C22
7	A	2402	CLR	C17-C20-C22-C23
10	C	1202	NAG	O5-C5-C6-O6
7	A	2404	CLR	C21-C20-C22-C23
7	A	2405	CLR	C21-C20-C22-C23
7	A	2404	CLR	C17-C20-C22-C23
7	A	2407	CLR	C17-C20-C22-C23
9	A	2409	PT5	C12-C10-O16-C8
8	A	2408	3PE	C32-C31-O31-C3
7	A	2405	CLR	C17-C20-C22-C23
10	C	1203	NAG	C8-C7-N2-C2
10	C	1203	NAG	O7-C7-N2-C2
8	A	2408	3PE	O32-C31-O31-C3
9	A	2409	PT5	C37-C38-C39-C40
9	A	2409	PT5	O17-C10-O16-C8
7	A	2407	CLR	C13-C17-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	A	2404	CLR	C20-C22-C23-C24
10	C	1203	NAG	C4-C5-C6-O6
7	A	2407	CLR	C20-C22-C23-C24
7	A	2402	CLR	C20-C22-C23-C24
8	A	2406	3PE	C22-C21-O21-C2
8	A	2408	3PE	C36-C37-C38-C39
8	A	2406	3PE	O22-C21-O21-C2
9	A	2409	PT5	C12-C13-C14-C15
10	C	1203	NAG	O5-C5-C6-O6
9	A	2409	PT5	C34-C35-C36-C37
9	A	2409	PT5	C10-C12-C13-C14
9	A	2409	PT5	C32-C33-C34-C35
7	A	2407	CLR	C16-C17-C20-C21
8	A	2406	3PE	C38-C39-C3A-C3B
8	A	2406	3PE	C39-C3A-C3B-C3C
7	A	2403	CLR	C21-C20-C22-C23
9	A	2409	PT5	C26-C27-C28-C29
7	A	2407	CLR	C16-C17-C20-C22
9	A	2409	PT5	C39-C40-C41-C42
9	A	2409	PT5	C31-C32-C33-C34
9	A	2409	PT5	C36-C37-C38-C39
8	A	2406	3PE	C32-C31-O31-C3
10	C	1202	NAG	C4-C5-C6-O6
9	A	2409	PT5	C8-C7-O13-P1
7	A	2405	CLR	C13-C17-C20-C22
8	A	2406	3PE	O32-C31-O31-C3
9	A	2409	PT5	C22-C23-C24-C25
9	A	2409	PT5	C35-C36-C37-C38
9	A	2409	PT5	O13-C7-C8-C9
7	A	2405	CLR	C16-C17-C20-C22
7	A	2405	CLR	C13-C17-C20-C21
8	A	2406	3PE	C3-C2-O21-C21
8	A	2406	3PE	C12-C11-O13-P
7	A	2405	CLR	C16-C17-C20-C21
8	A	2406	3PE	O11-C1-C2-O21
9	A	2409	PT5	O13-C7-C8-O16
9	A	2409	PT5	O16-C8-C9-O18
9	A	2409	PT5	C7-C8-C9-O18
8	A	2406	3PE	C11-O13-P-O11
10	C	1201	NAG	C3-C2-N2-C7
9	A	2409	PT5	C7-C8-O16-C10
9	A	2409	PT5	C5-O5-P5-O51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	A	2406	3PE	O11-C1-C2-C3
7	A	2404	CLR	C16-C17-C20-C22
8	A	2406	3PE	C2-C1-O11-P
9	A	2409	PT5	C2-C1-O1-P1
8	A	2408	3PE	O21-C2-C3-O31
9	A	2409	PT5	C19-C20-C21-C22
9	A	2409	PT5	C4-O4-P4-O42
10	C	1201	NAG	C1-C2-N2-C7
8	A	2408	3PE	C3B-C3C-C3D-C3E
8	A	2406	3PE	C35-C36-C37-C38
8	A	2406	3PE	C3B-C3C-C3D-C3E
9	A	2409	PT5	C1-O1-P1-O12
8	A	2408	3PE	O31-C31-C32-C33
9	A	2409	PT5	C4-O4-P4-O41
9	A	2409	PT5	C4-O4-P4-O43
9	A	2409	PT5	O16-C10-C12-C13
7	A	2404	CLR	C13-C17-C20-C21
7	A	2404	CLR	C13-C17-C20-C22
7	A	2405	CLR	C22-C23-C24-C25
8	A	2408	3PE	O32-C31-C32-C33
9	A	2409	PT5	O17-C10-C12-C13
7	A	2405	CLR	C23-C24-C25-C27
8	A	2408	3PE	C32-C33-C34-C35

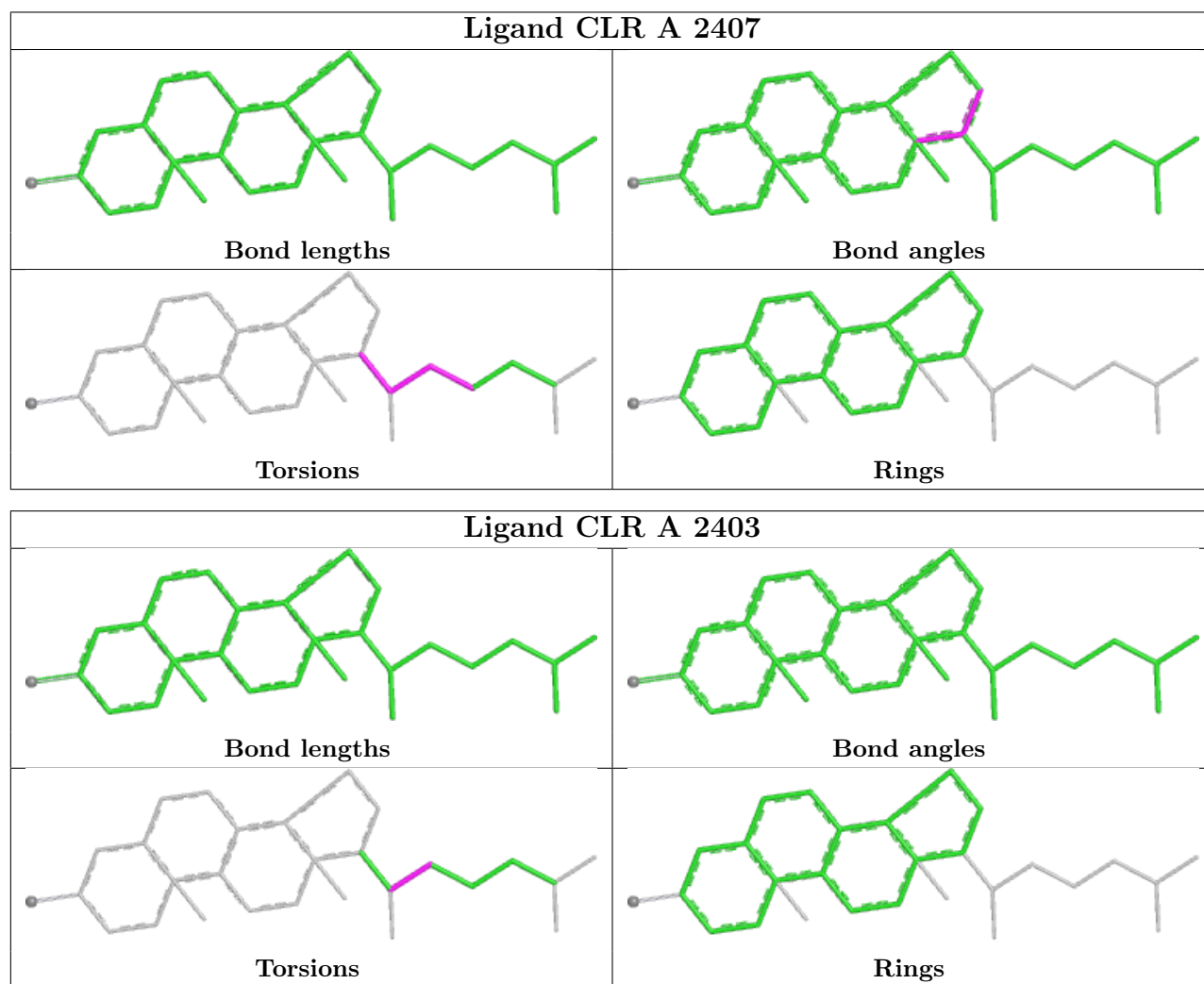
There are no ring outliers.

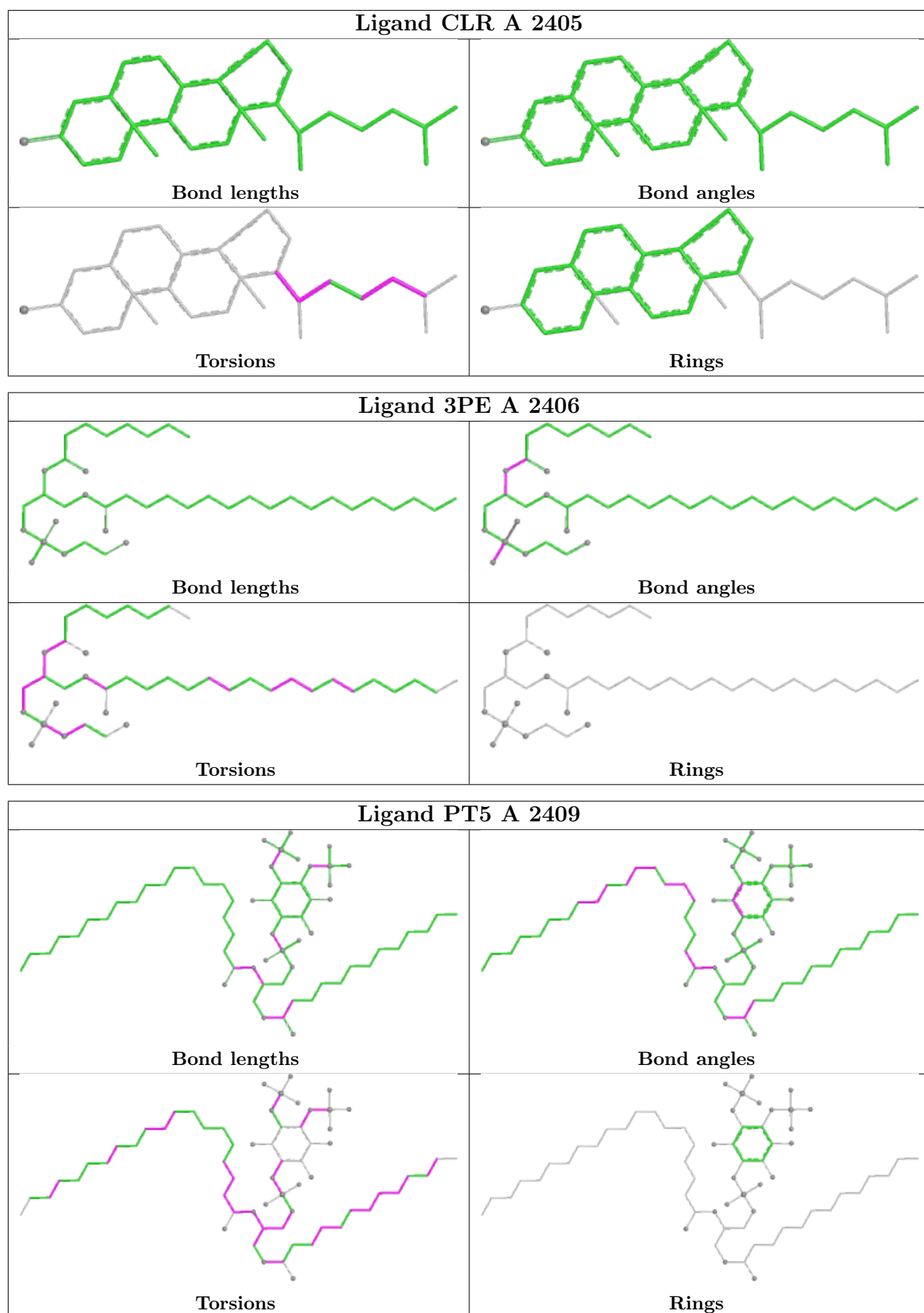
7 monomers are involved in 18 short contacts:

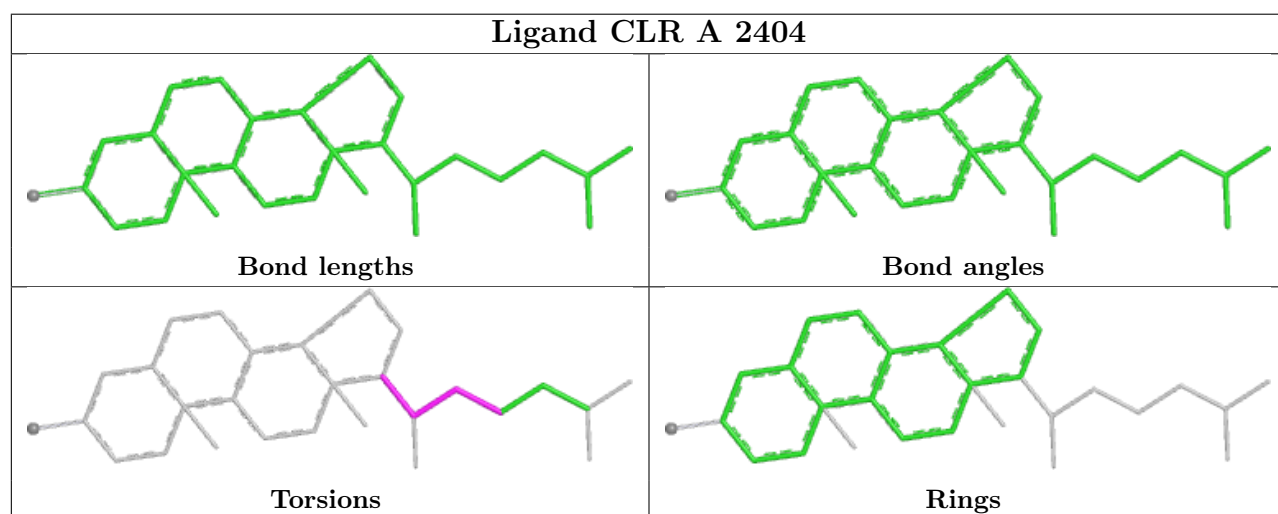
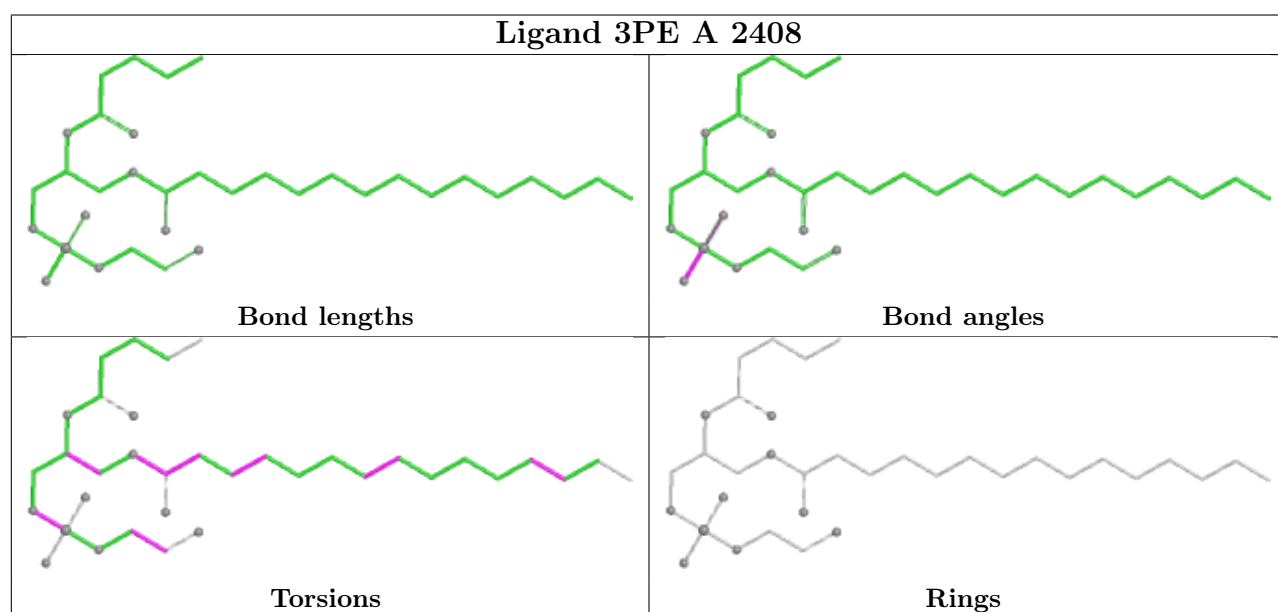
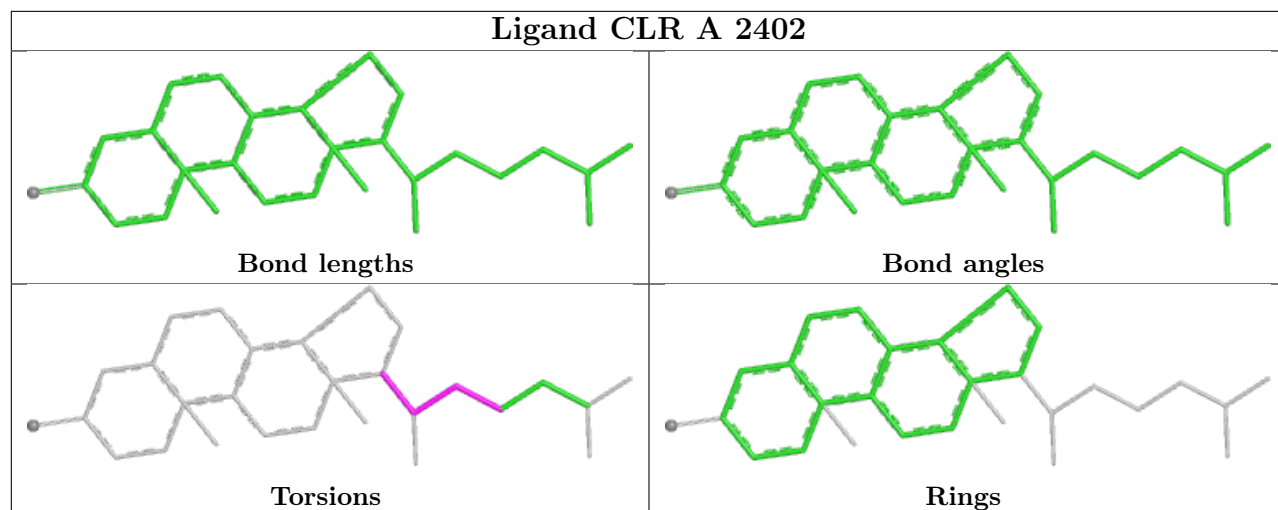
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2407	CLR	2	0
10	C	1202	NAG	2	0
7	A	2405	CLR	1	0
8	A	2406	3PE	1	0
9	A	2409	PT5	5	0
7	A	2402	CLR	5	0
7	A	2404	CLR	2	0

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

There are no chain breaks in this entry.

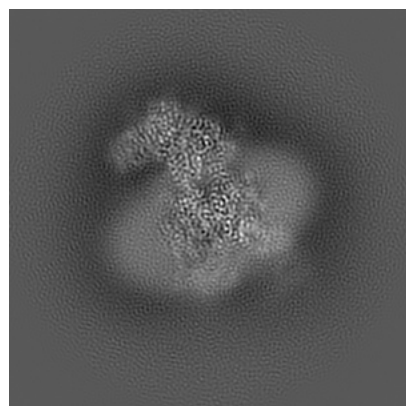
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28529. These allow visual inspection of the internal detail of the map and identification of artifacts.

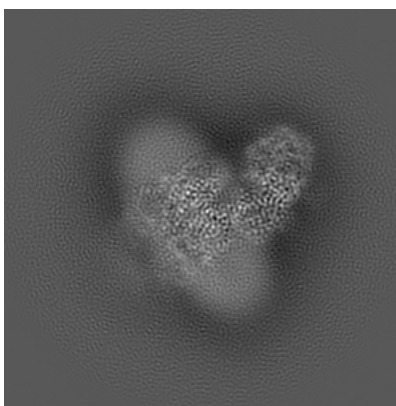
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

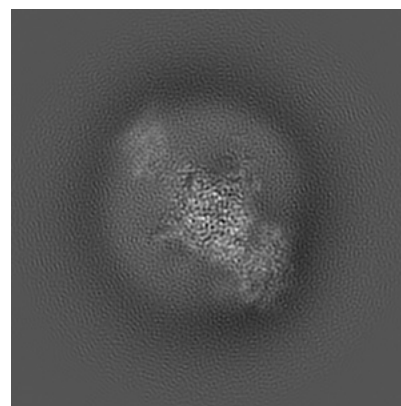
#### 6.1.1 Primary map



X

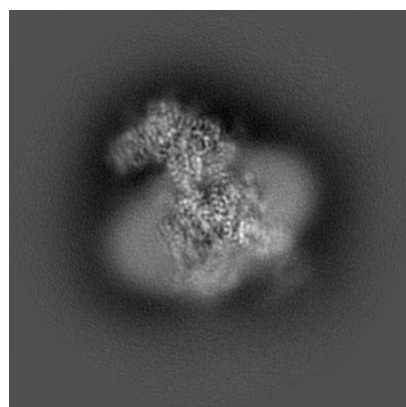


Y

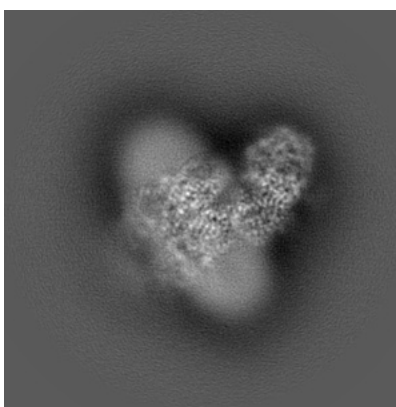


Z

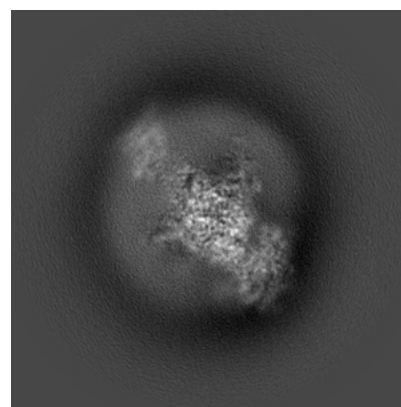
#### 6.1.2 Raw map



X



Y

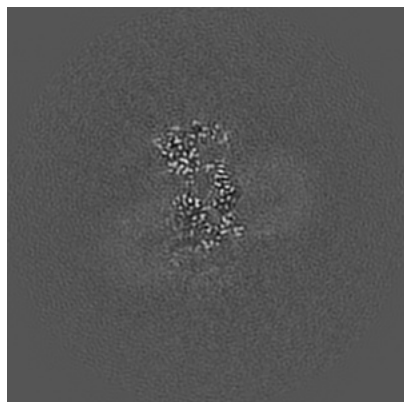


Z

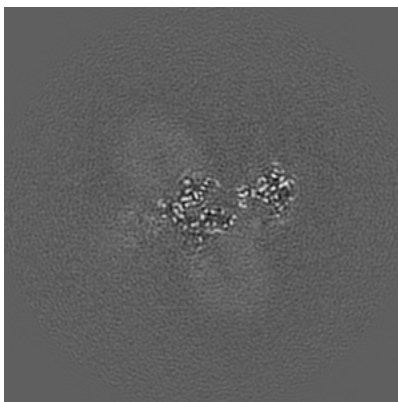
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

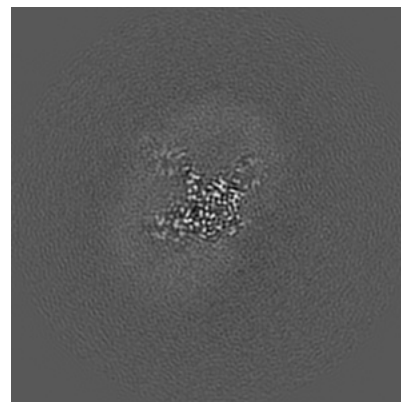
### 6.2.1 Primary map



X Index: 140

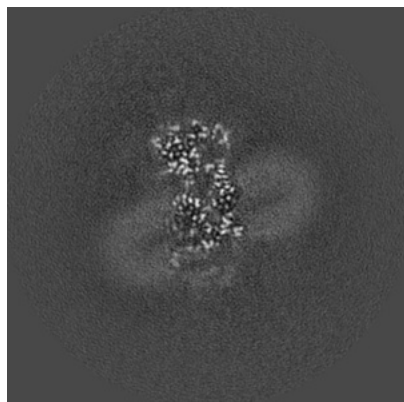


Y Index: 140

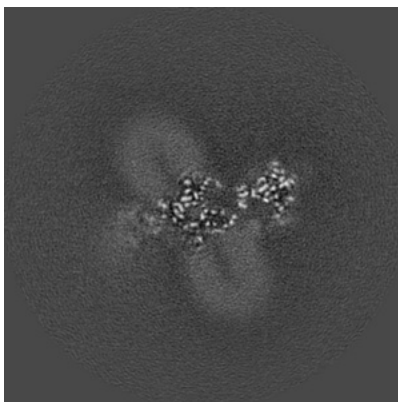


Z Index: 140

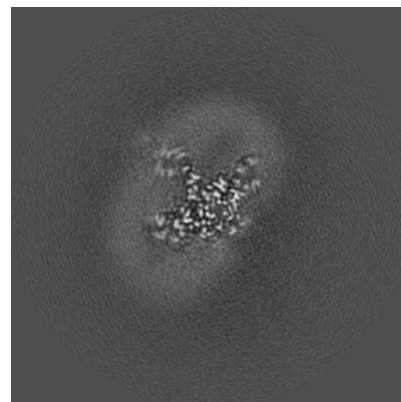
### 6.2.2 Raw map



X Index: 140



Y Index: 140

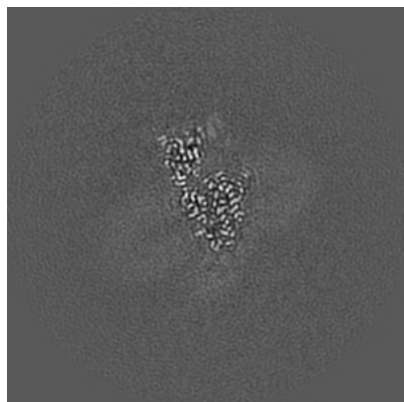


Z Index: 140

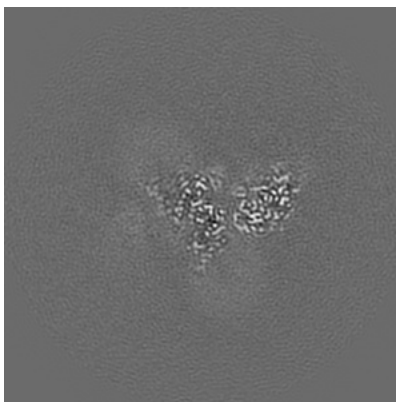
The images above show central slices of the map in three orthogonal directions.

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

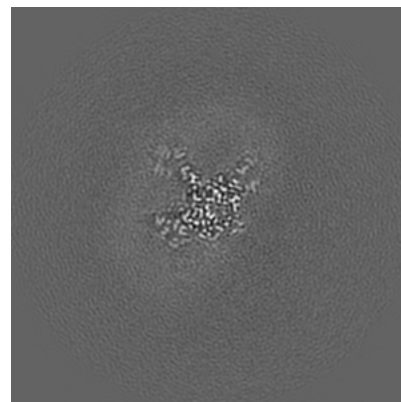
### 6.3.1 Primary map



X Index: 130

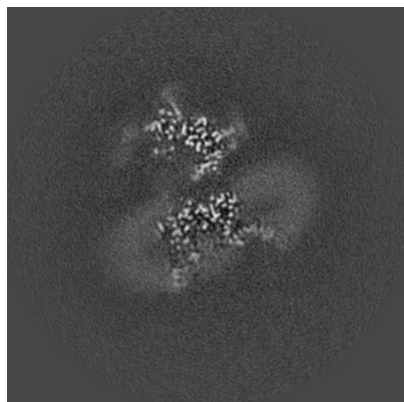


Y Index: 132

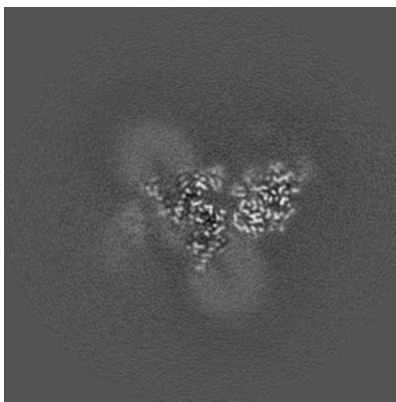


Z Index: 141

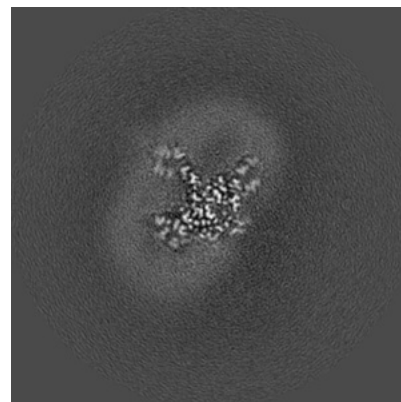
### 6.3.2 Raw map



X Index: 149



Y Index: 132

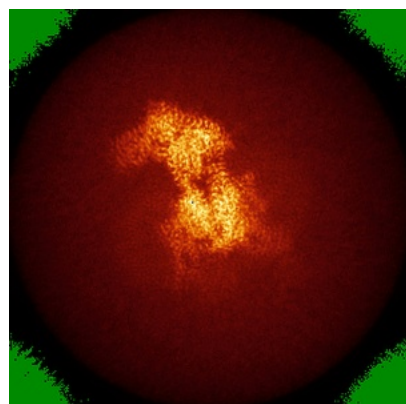


Z Index: 141

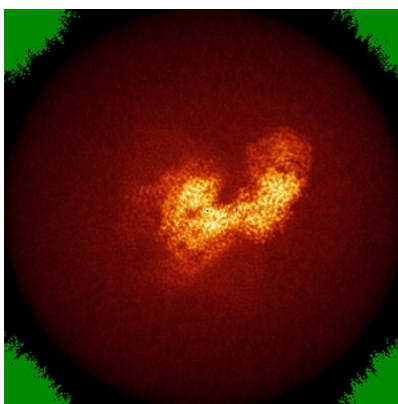
The images above show the largest variance slices of the map in three orthogonal directions.

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

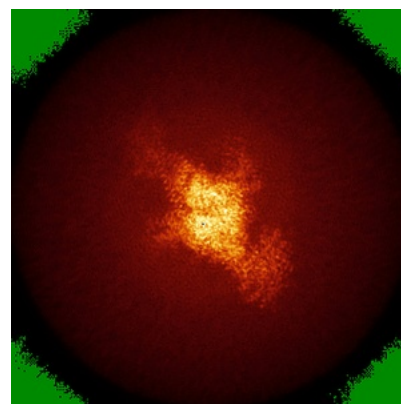
### 6.4.1 Primary map



X

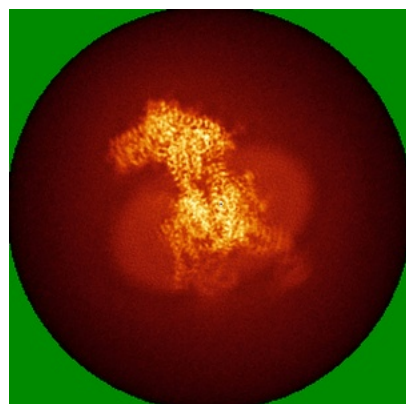


Y

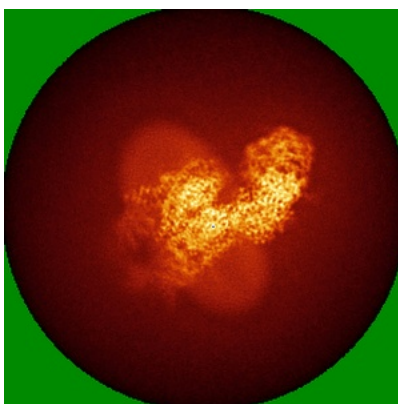


Z

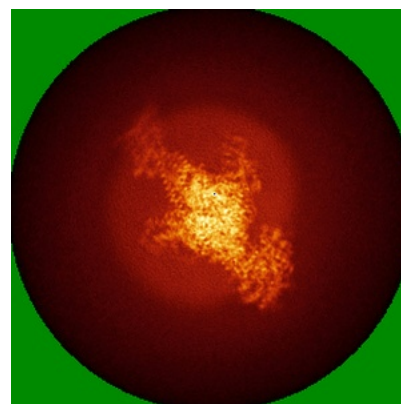
### 6.4.2 Raw map



X



Y

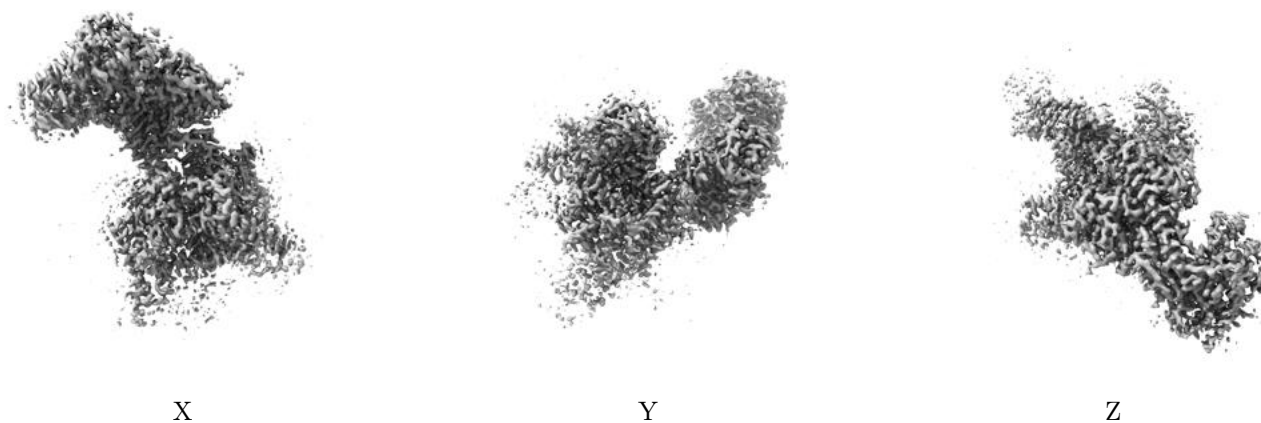


Z

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 0.03. 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.

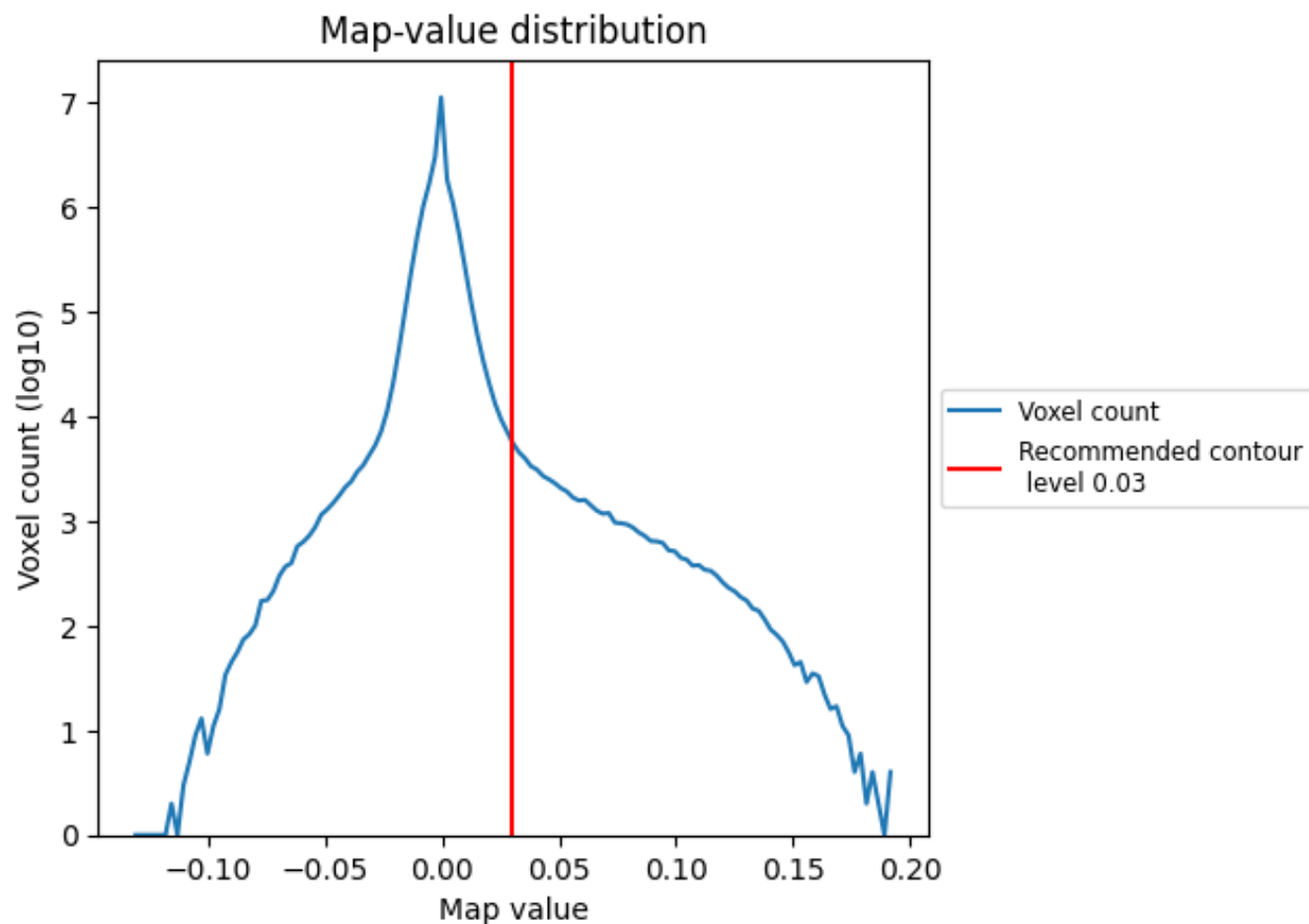
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

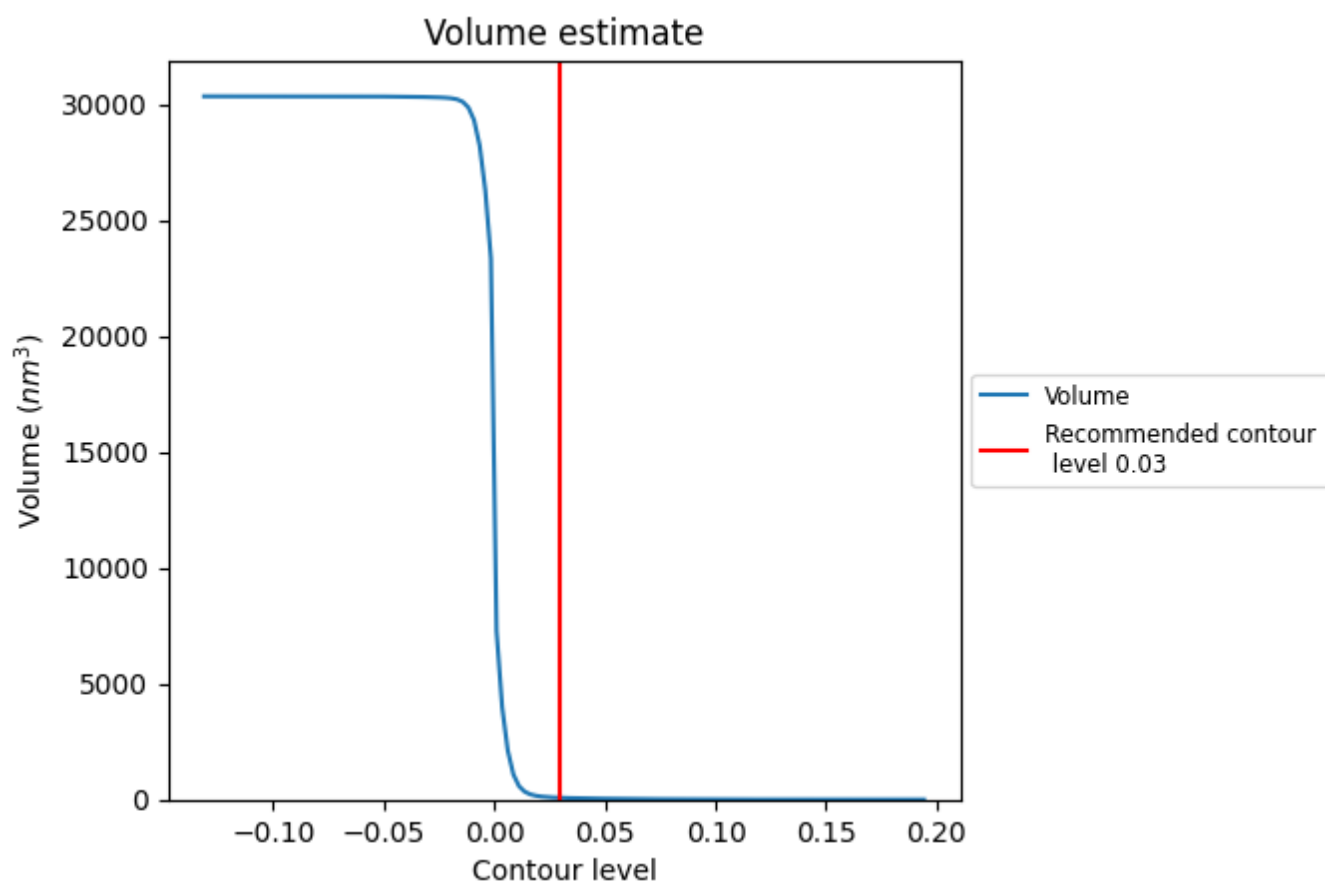
This section contains the results of statistical analysis of the map.

### 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.

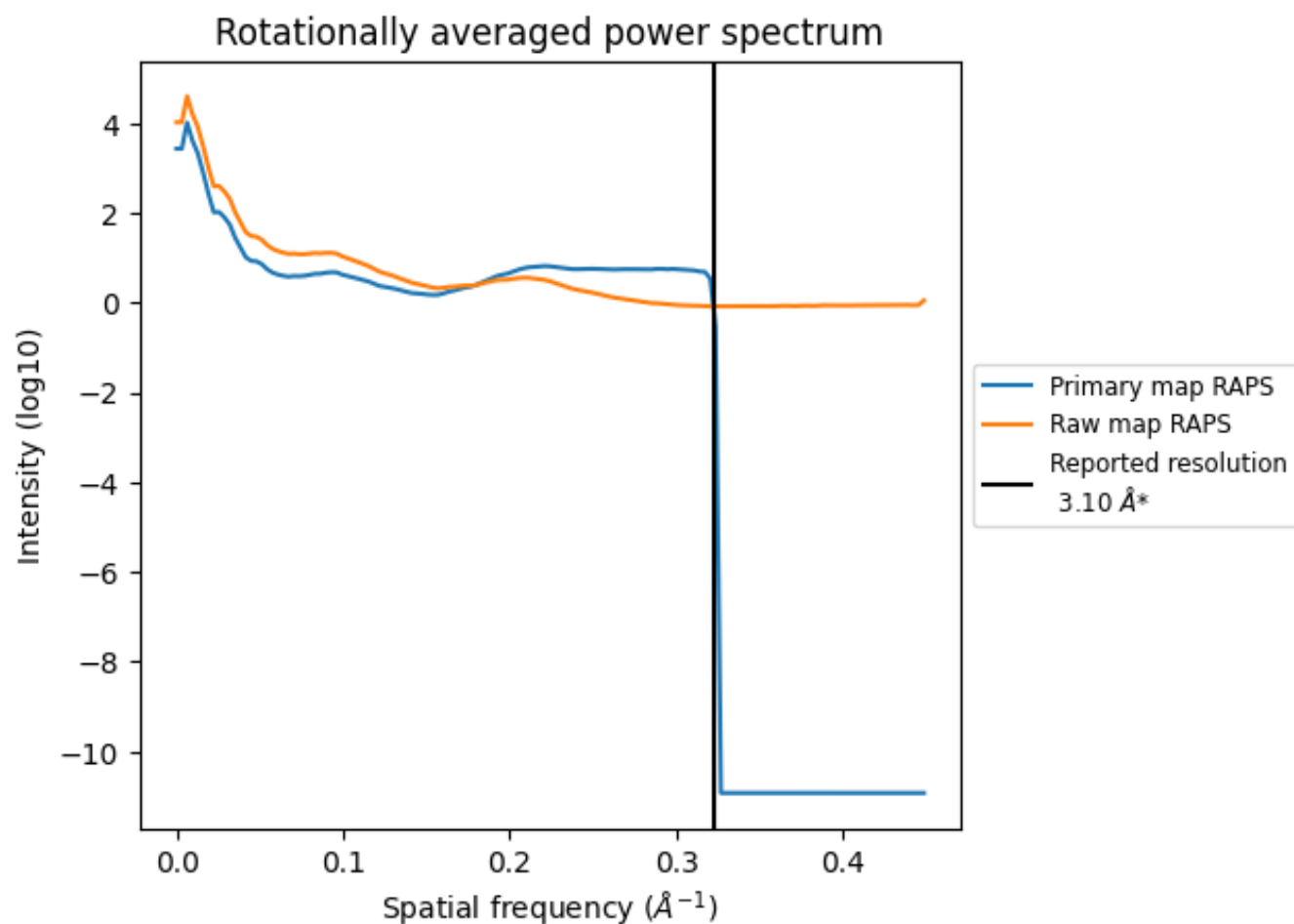
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77  $\text{nm}^3$ ; this corresponds to an approximate mass of 69 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 ⓘ

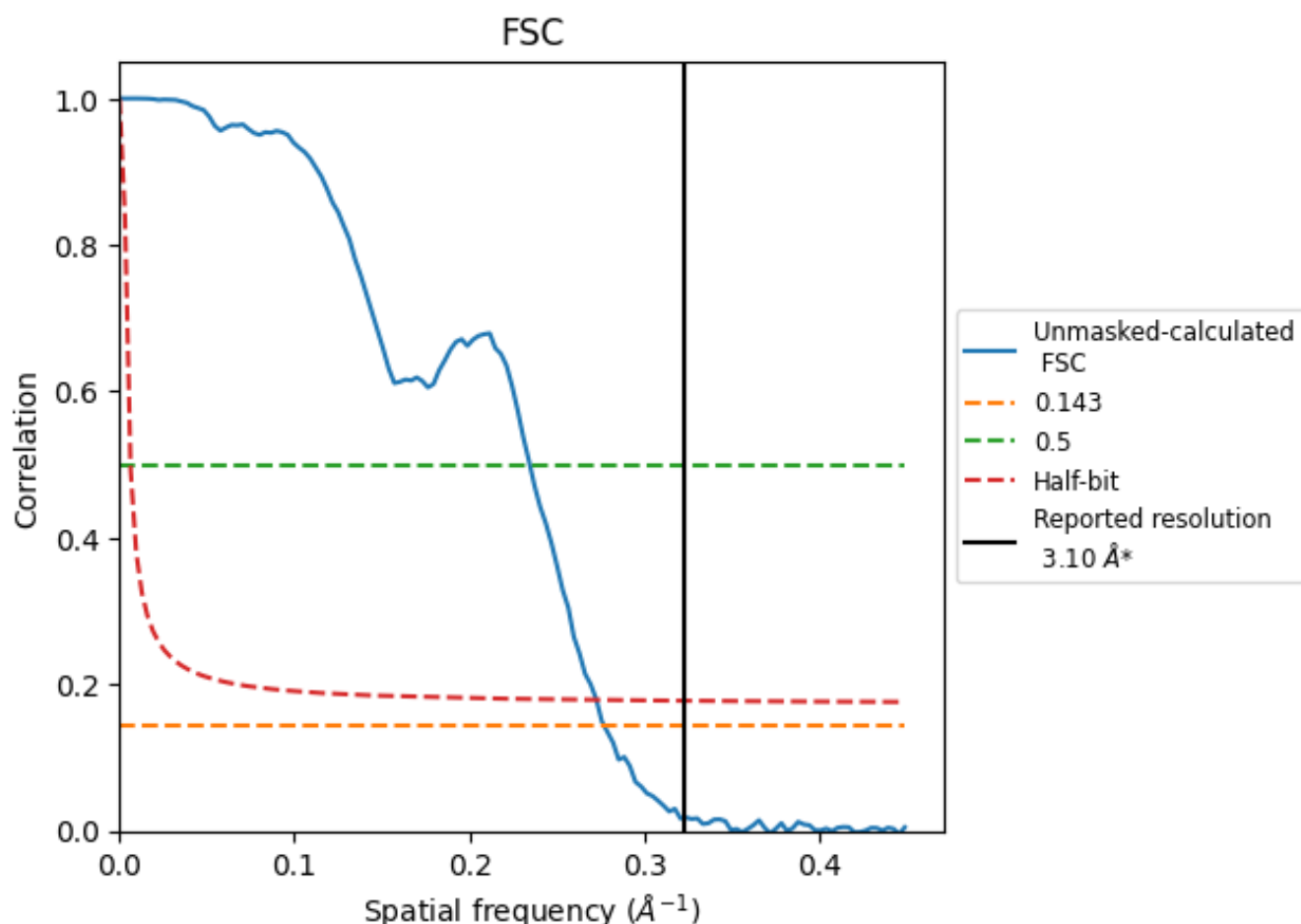


\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

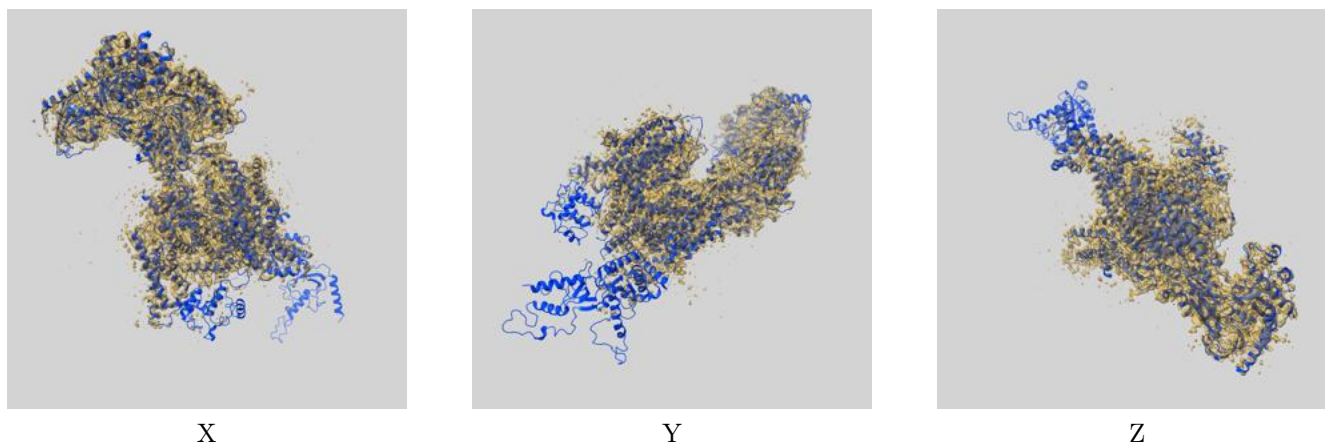
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.67

\*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 3.61 differs from the reported value 3.1 by more than 10 %

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

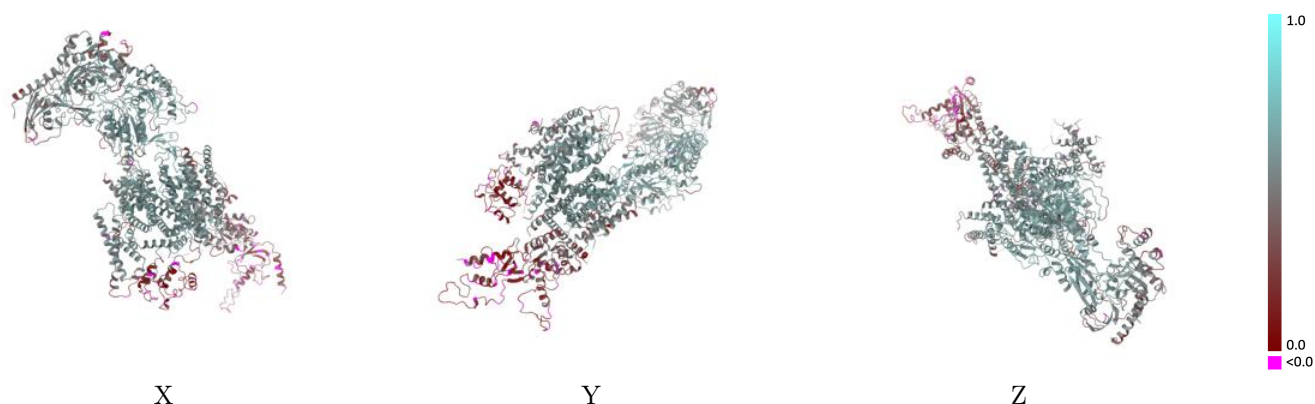
This section contains information regarding the fit between EMDB map EMD-28529 and PDB model 8EPL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



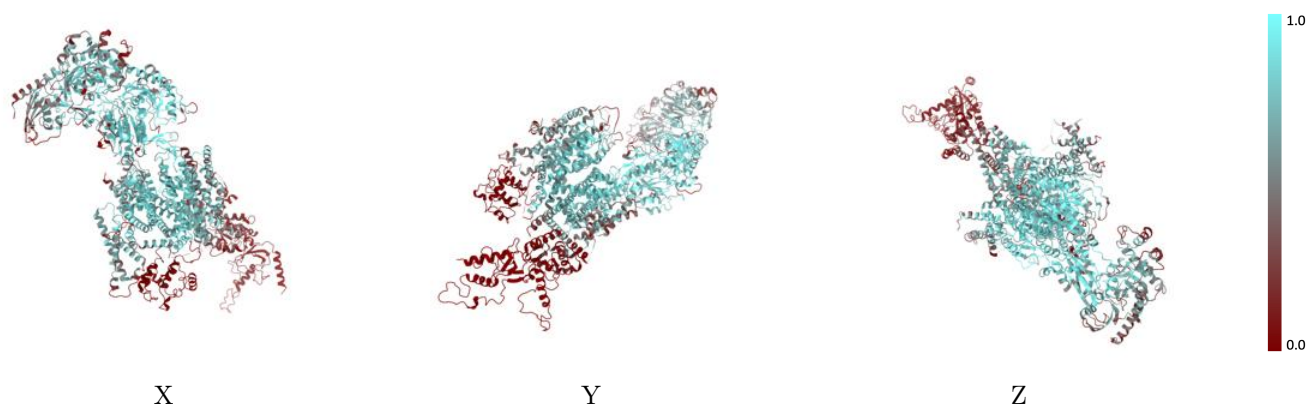
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



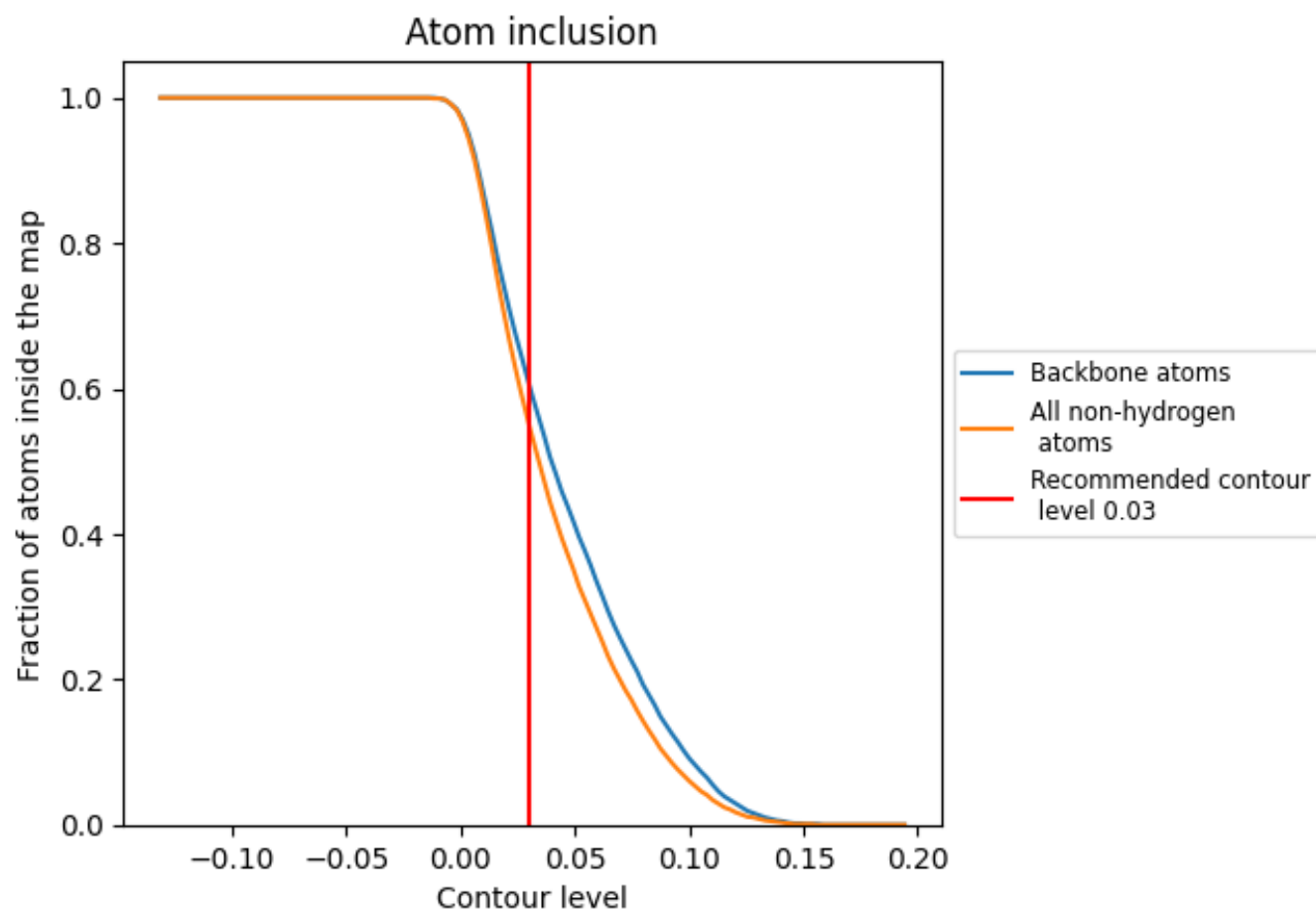
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 55% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5500	 0.4720
A	 0.5920	 0.4900
B	 0.0360	 0.2270
C	 0.6710	 0.5310
D	 0.3570	 0.4250
E	 0.0710	 0.2490
F	 0.4110	 0.4220
G	 0.2140	 0.4810
H	 0.2860	 0.3200

