



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 02:27 AM JST

PDB ID : 8WE8  
EMDB ID : EMD-37474  
Title : Human L-type voltage-gated calcium channel Cav1.2 in the presence of cal-ciseptine, amlodipine and pinaverium at 2.9 Angstrom resolution  
Authors : Gao, S.; Yao, X.; Yan, N.  
Deposited on : 2023-09-17  
Resolution : 2.90 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

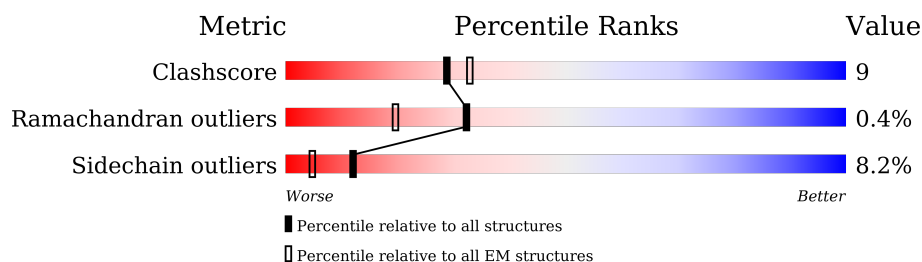
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	2201	<div> <div>8%</div> <div>42%</div> <div>14%</div> <div>•</div> <div>43%</div> </div>
2	D	1103	<div> <div>•</div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
3	C	484	<div> <div>56%</div> <div>45%</div> <div>19%</div> <div>•</div> <div>33%</div> </div>
4	B	60	<div> <div>52%</div> <div>47%</div> <div>45%</div> <div>8%</div> </div>
5	E	3	<div> <div>33%</div> <div>67%</div> <div>33%</div> </div>
6	F	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>
6	H	2	<div> <div>50%</div> <div>100%</div> </div>
6	I	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	4	<div><div></div><div>50%</div><div></div><div>50%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21309 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 L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1261	Total	C	N	O	S	0	0
			10183	6695	1660	1765	63		

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

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

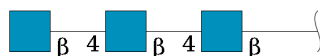
- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

- Molecule 4 is a protein called Calciseptin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	60	Total	C	N	O	S	0	0
			486	299	90	87	10		

- Molecule 5 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
5	E	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 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
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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.

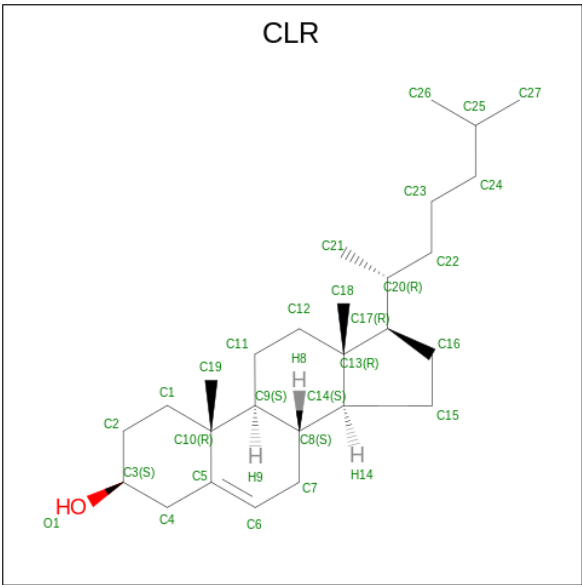


Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	
8	D	1	Total	Ca	0
			1	1	

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



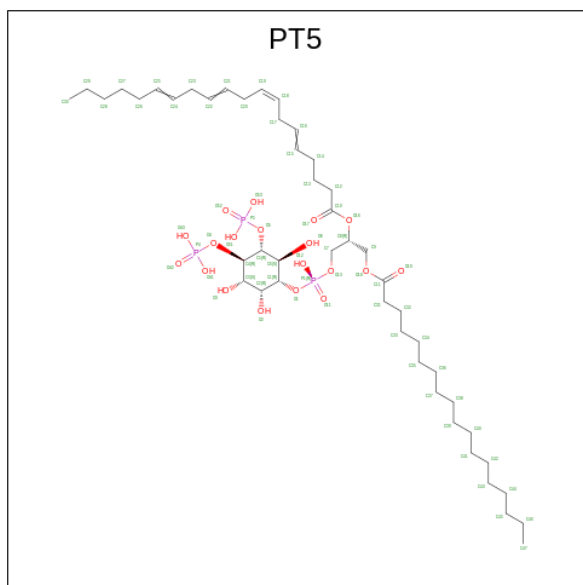
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	B	1	Total	C	O	0
			28	27	1	

- 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>).



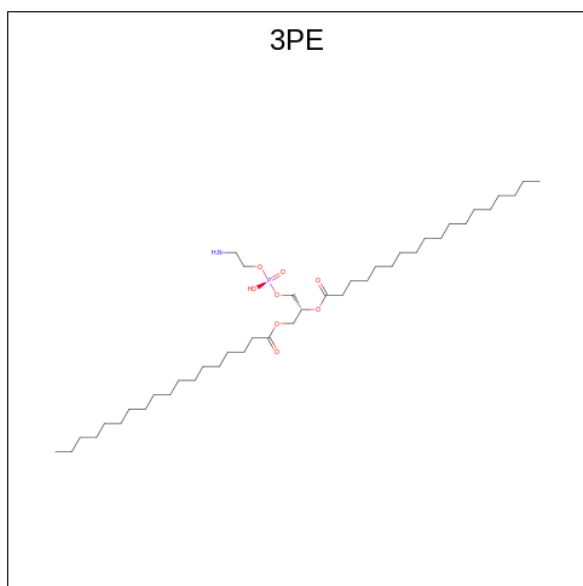
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	

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



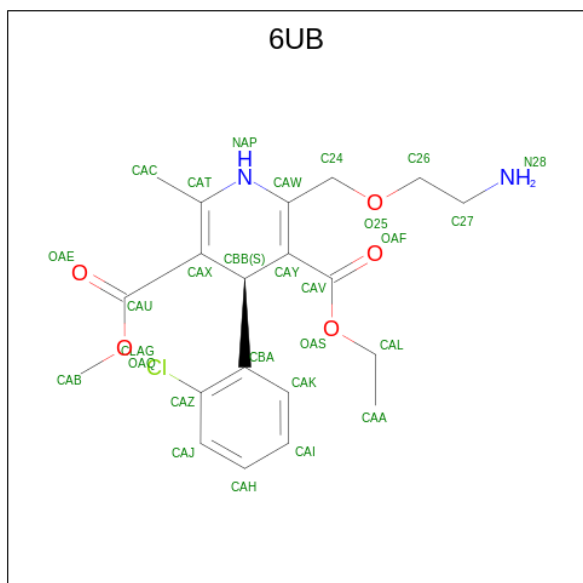
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			63	41	19	3	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 13 is amlodipine (three-letter code: 6UB) (formula:  $C_{20}H_{25}ClN_2O_5$ ).

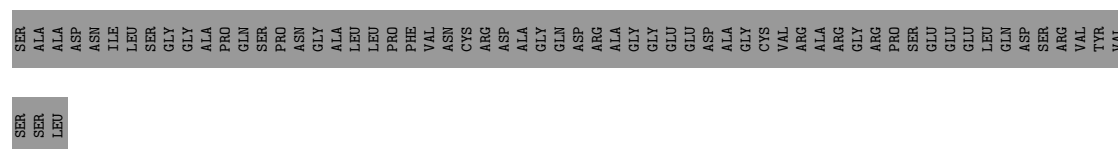




Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
13	A	1	28	20	1	2	5	0

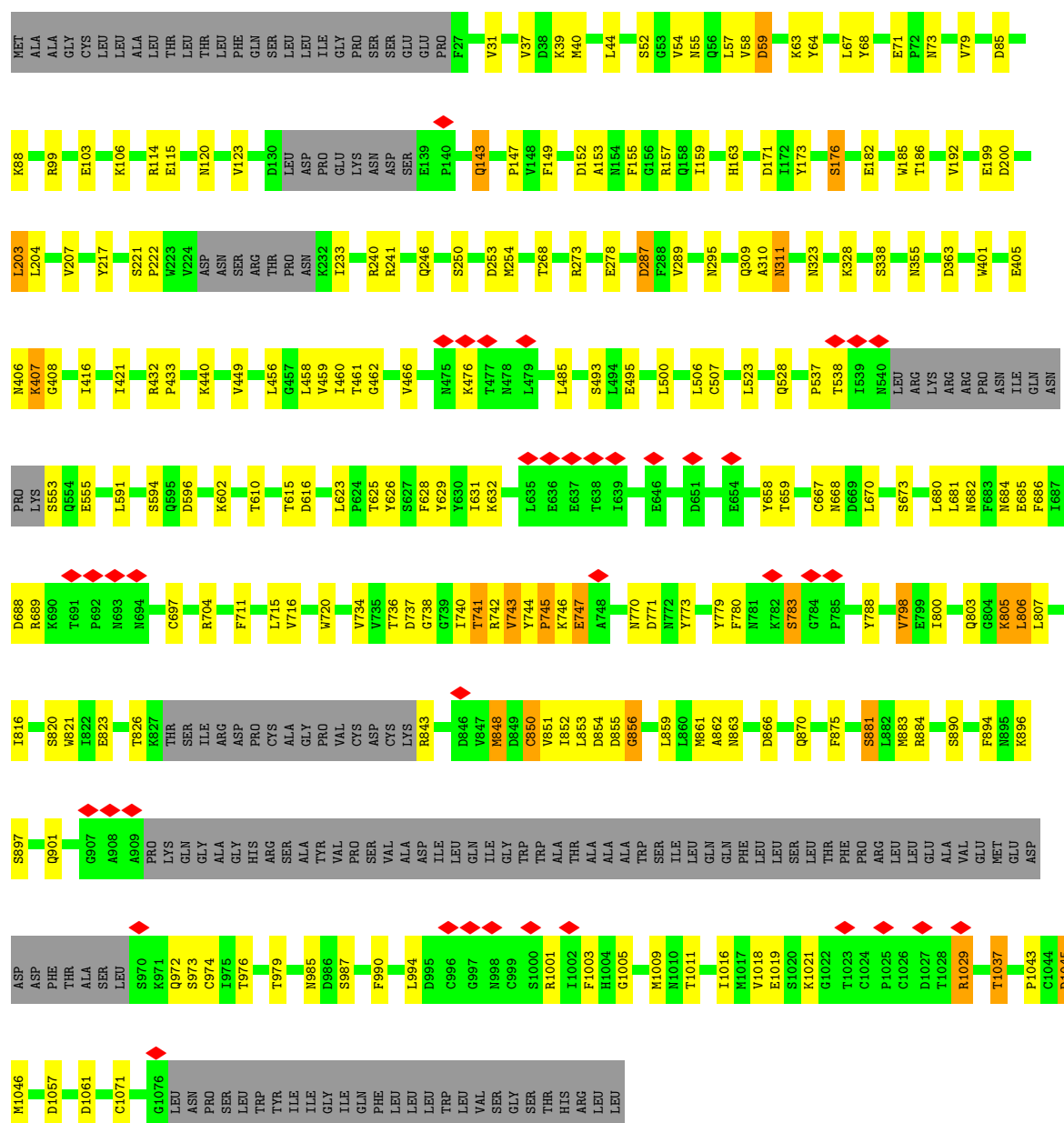


LEU	THR	THR	LEU	SER	PHE	R1619	G1558	T1449	GLU	M1258	I1172	I1006	T900
MET	TYR	TYR	SER	GLU	LYS	I1620	R1559	F1450	VAL	M1271	I1181	I1007	F902
VAL	VAL	VAL	ASP	ASP	ARG	K1621	I1560	P1451	ASN	I1273	F1185	Q1008	T903
GLY	LYS	LYS	ILE	ILE	LYS	T1622	K1561	R1459	ALA	I1274	V1185	S1009	N904
ALA	ASN	ASN	GLU	GLU	GLN	E1623	H1562	T1462	HIS	L1274	V1185	S1009	L905
GLY	GLN	GLN	GLY	GLY	GLY	G1624	L1563	T1462	THR	L1274	F1189	A1010	L906
HIS	HIS	HIS	VAL	VAL	VAL	M1625	D1564	A1465	GLN	E1285	Q1190	L1017	L907
TRP	ASP	ASP	PRO	PRO	PRO	L1626	V1565	Q1467	CYS	M1286	E1191	R1018	F908
GLN	GLY	GLY	GLY	GLY	GLY	E1627	T1567	D1468	SER	I1287	Q1192	L1019	L912
GLY	GLY	GLY	GLY	GLY	GLY	Q1628	L1568	G1476	PRO	L1288	G1193	V1019	S916
ASP	ASP	ASP	PRO	PRO	PRO	A1629	L1569	C1479	MET	K1289	E1194	L1018	L917
ASP	ASP	ASP	SER	SER	SER	M1630	L1570	C1479	ASN	L1290	E1196	L1020	
GLY	GLY	GLY	GLN	GLN	GLN	E1631	R1571	E1482	ASN	A1291	Q1195	R1021	
GLY	GLY	GLY	VAL	VAL	VAL	L1632	I1572	E1483	GLU	K1294	Y1197	R1024	V923
ALA	ALA	ALA	ASN	ASN	ASN	L1633	I1573	E1484	GLU	P1295	K1198	T926	H925
ALA	ALA	ALA	ASN	ASN	ASN	R1634	Q1574	PRO	ASN	N1199	R1027	S927	S927
ALA	ALA	ALA	ASN	ASN	ASN	A1635	P1575	ASN	ARG	Y1298	A1028	F928	N929
ALA	ALA	ALA	ASN	ASN	ASN	T1636	L1576	SER	ILE	P1302	C1200	A1032	N930
ALA	ALA	ALA	ASN	ASN	ASN	I1637	G1577	T1489	ILE	M1303	E1201	A1032	H931
ALA	ALA	ALA	ASN	ASN	ASN	K1638	F1578	E1490	THR	M1304	L1202	V1042	T961
ALA	ALA	ALA	ASN	ASN	ASN	K1639	G1579	G1491	THR	L1309	D1203	I1049	S962
ALA	ALA	ALA	ASN	ASN	ASN	I1640	K1580	E1492	THR	L1312	K1204	T1068	T965
ALA	ALA	ALA	ASN	ASN	ASN	W1641	L1581	Y1503	THR	I1315	M1205	Q1069	L966
ALA	ALA	ALA	ASN	ASN	ASN	R1643	C1582	L1514	THR	I1315	Q1206	K1072	E967
ALA	ALA	ALA	ASN	ASN	ASN	T1644	H1584	L1514	THR	E1322	R1207	G1073	T968
ALA	ALA	ALA	ASN	ASN	ASN	S1645	R1585	V1520	THR	T1323	Q1208	K1074	T969
ALA	ALA	ALA	ASN	ASN	ASN	M1646	V1586	M1524	THR	ASN	E1211	L970	L970
ALA	ALA	ALA	ASN	ASN	ASN	K1647	V1587	M1524	THR	HIS	Y1212	T1095	A971
ALA	ALA	ALA	ASN	ASN	ASN	L1648	C1588	F1527	THR	PHE	A1213	G1099	N972
ALA	ALA	ALA	ASN	ASN	ASN	L1649	K1589	L1530	THR	CYS	L1214	V1101	T973
ALA	ALA	ALA	ASN	ASN	ASN	ASP	R1590	T1531	THR	ASP	A1216	G976	A974
ALA	ALA	ALA	ASN	ASN	ASN	GLN	L1591	R1532	THR	ALA	P1104	ALA	ALA
ALA	ALA	ALA	ASN	ASN	ASN	VAL	L1591	D1533	THR	ASN	K1115	LEU	LEU
ALA	ALA	ALA	ASN	ASN	ASN	VAL	V1592	W1534	THR	THR	F1116	HIS	HIS
ALA	ALA	ALA	ASN	ASN	ASN	PRO	S1593	S1535	THR	ASP	D1117	LYS	LYS
ALA	ALA	ALA	ASN	ASN	ASN	ALA	M1594	S1535	THR	ASP	L1122	GLY	GLY
ALA	ALA	ALA	ASN	ASN	ASN	GLY	M1595	D1543	THR	ALA	M1126	SER	SER
ALA	ALA	ALA	ASN	ASN	ASN	ASP	M1596	E1544	THR	LEU	W1137	PHE	PHE
ALA	ALA	ALA	ASN	ASN	ASN	ASP	P1597	F1545	THR	VAL	K1225	CYS	CYS
ALA	ALA	ALA	ASN	ASN	ASN	VAL	L1598	K1546	THR	VAL	M1224	R986	
ALA	ALA	ALA	ASN	ASN	ASN	THR	M1599	R1547	THR	GLY	M1226	L994	L994
ALA	ALA	ALA	ASN	ASN	ASN	VAL	S1600	L1548	THR	GLY	Q1227	L995	L995
ALA	ALA	ALA	ASN	ASN	ASN	GLY	D1601	W1549	THR	ILE	H1228	V996	V996
ALA	ALA	ALA	ASN	ASN	ASN	LYS	G1602	A1550	THR	VAL	Q1229	V997	V997
ALA	ALA	ALA	ASN	ASN	ASN	PHE	G1603	E1551	THR	ASP	S1147	S998	S998
ALA	ALA	ALA	ASN	ASN	ASN	THR	T1603	E1551	THR	ALA	K1231	D1151	L1001
ALA	ALA	ALA	ASN	ASN	ASN	ALA	V1604	P1554	THR	ALA	W1233	R1159	I1002
ALA	ALA	ALA	ASN	ASN	ASN	PHE	M1605	E1556	THR	THR	V1236	S1003	S1003
ALA	ALA	ALA	ASN	ASN	ASN	LEU	F1606	K1557	THR	GLY	M1245		
ALA	ALA	ALA	ASN	ASN	ASN	ILE	M1607		THR	GLY	I1249		
ALA	ALA	ALA	ASN	ASN	ASN	GLN	A1608		THR	GLY	I1254		
ALA	ALA	ALA	ASN	ASN	ASN	TYR	T1609		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN	PHE	L1610		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN	ARG	F1611		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN	LYS			THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN		V1614		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN		R1615		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN		T1616		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN		A1617		THR	GLY			
ALA	ALA	ALA	ASN	ASN	ASN		L1618		THR	GLY			



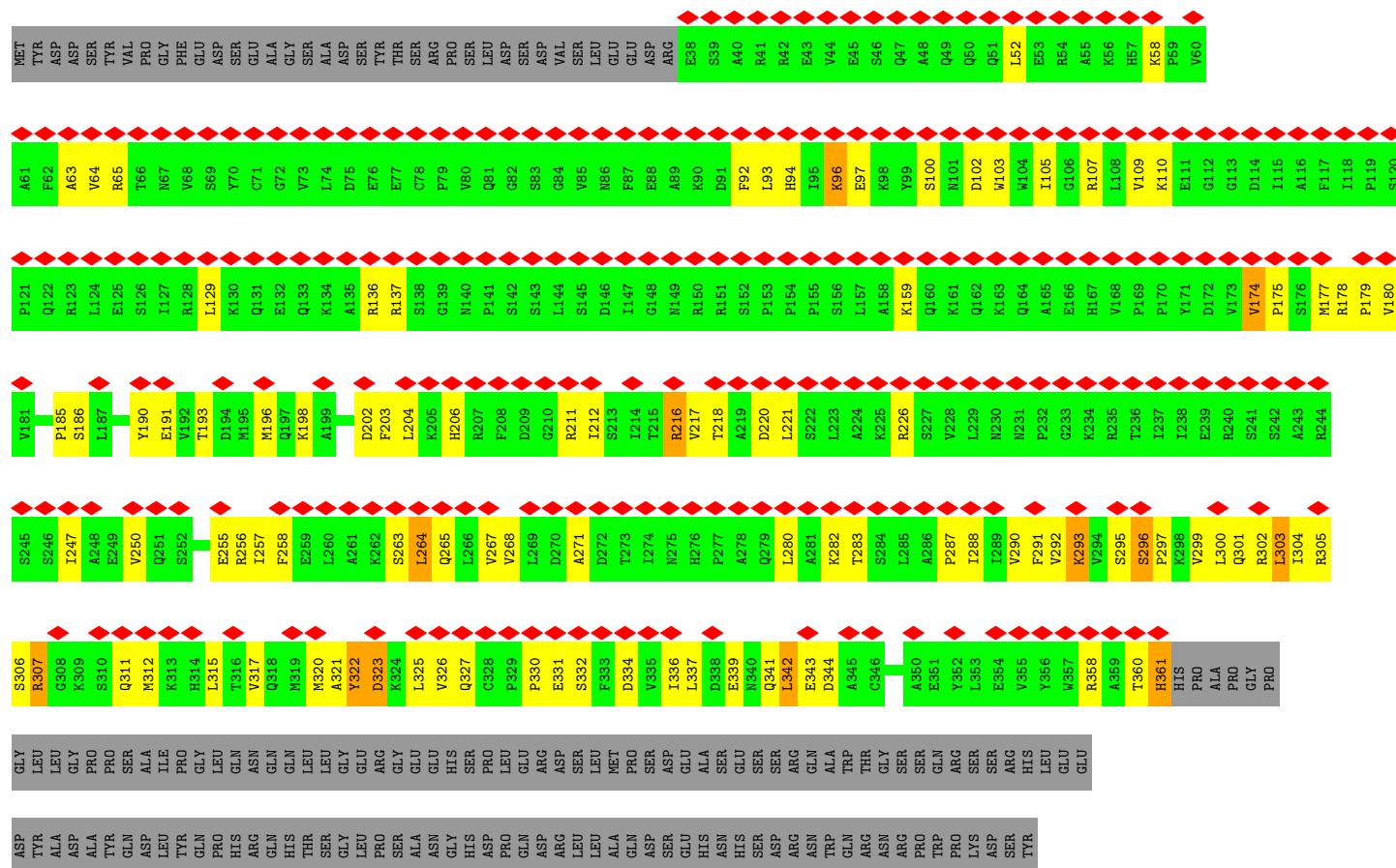
• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D: 

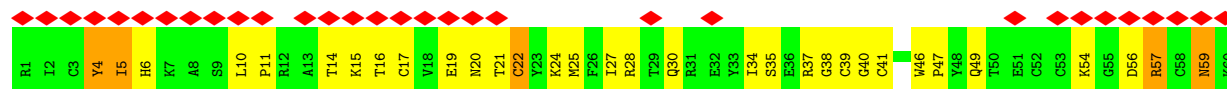


• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3

Chain C: 



### • Molecule 4: Calciseptin



### • 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



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





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



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



- Molecule 7: 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	118337	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	4.895	Depositor
Minimum map value	-3.503	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.45	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, PT5, CLR, NAG, CA, 6UB

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	0.29	0/10414	0.49	0/14109
2	D	0.25	0/7728	0.47	0/10477
3	C	0.24	0/2624	0.50	0/3544
4	B	0.29	0/496	0.65	0/664
All	All	0.27	0/21262	0.49	0/28794

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10183	0	10404	198	0
2	D	7570	0	7369	119	0
3	C	2575	0	2619	60	0
4	B	486	0	474	21	0
5	E	42	0	37	2	0
6	F	28	0	25	1	0
6	H	28	0	25	0	0
6	I	28	0	25	0	0
7	G	56	0	49	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	A	112	0	184	7	0
9	B	28	0	46	2	0
10	A	14	0	13	0	0
10	D	28	0	26	1	0
11	A	63	0	67	1	0
12	A	38	0	50	0	0
13	A	28	0	0	0	0
All	All	21309	0	21413	394	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 (394) 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)
4:B:4:TYR:H	4:B:57:ARG:HH12	1.09	0.99
1:A:1236:VAL:HG21	1:A:1289:LYS:HG2	1.49	0.93
1:A:1290:LEU:HD13	1:A:1298:TYR:HD2	1.45	0.82
2:D:850:CYS:SG	2:D:863:ASN:ND2	2.58	0.77
1:A:681:GLU:OE2	1:A:681:GLU:N	2.20	0.75
3:C:322:TYR:CE1	3:C:326:VAL:HG21	2.22	0.74
1:A:1221:ARG:HG2	1:A:1551:GLU:HA	1.68	0.74
3:C:52:LEU:HD21	3:C:105:ILE:HG12	1.69	0.74
1:A:1573:GLN:HG2	1:A:1575:PRO:HD2	1.71	0.73
1:A:136:ALA:HA	1:A:139:VAL:HG12	1.71	0.72
1:A:365:TRP:HE1	1:A:1462:THR:HG21	1.55	0.71
1:A:143:ILE:HG22	1:A:159:LEU:HD11	1.72	0.71
4:B:22:CYS:HA	4:B:39:CYS:HA	1.73	0.71
1:A:1434:ALA:HB2	1:A:1479:CYS:HA	1.73	0.70
2:D:71:GLU:HG3	2:D:632:LYS:HE3	1.75	0.68
2:D:854:ASP:O	2:D:856:GLY:N	2.25	0.68
3:C:330:PRO:O	3:C:332:SER:N	2.25	0.68
1:A:1207:ARG:HH21	1:A:1636:ILE:HG12	1.59	0.68
3:C:295:SER:OG	3:C:296:SER:N	2.28	0.67
1:A:1459:ARG:HH21	1:A:1465:ALA:HB3	1.59	0.66
1:A:1482:GLU:OE2	1:A:1482:GLU:N	2.23	0.66
1:A:299:TYR:HA	1:A:308:PRO:HD2	1.77	0.66
1:A:1290:LEU:HD22	1:A:1298:TYR:CE2	2.31	0.66
1:A:1290:LEU:HD13	1:A:1298:TYR:CD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:VAL:HG12	1:A:1292:ALA:HB2	1.79	0.65
2:D:853:LEU:HD21	2:D:875:PHE:CD2	2.32	0.64
3:C:360:THR:O	3:C:361:HIS:ND1	2.30	0.64
4:B:4:TYR:N	4:B:57:ARG:HH12	1.89	0.64
1:A:1605:MET:HE1	1:A:1607:ASN:HB2	1.79	0.63
1:A:1226:ASN:C	1:A:1228:HIS:H	2.01	0.63
1:A:426:GLU:OE2	1:A:429:GLN:NE2	2.32	0.63
2:D:240:ARG:NH2	2:D:278:GLU:O	2.32	0.63
2:D:629:TYR:HB2	2:D:807:LEU:HD21	1.80	0.63
1:A:1440:GLU:HG3	1:A:1468:ASP:HB3	1.80	0.62
3:C:177:MET:HB2	3:C:264:LEU:HA	1.80	0.62
3:C:293:LYS:HD2	3:C:295:SER:H	1.65	0.62
1:A:1449:THR:HG22	1:A:1451:PRO:HD2	1.79	0.62
1:A:298:CYS:HB2	1:A:309:ALA:HB2	1.82	0.62
1:A:1572:ILE:HD12	1:A:1577:GLY:HA3	1.82	0.61
2:D:994:LEU:N	2:D:1001:ARG:O	2.31	0.61
1:A:201:ILE:O	1:A:205:VAL:HG23	2.00	0.61
1:A:609:LYS:HG2	1:A:610:ILE:H	1.66	0.61
2:D:254:MET:HB3	2:D:289:VAL:HG23	1.83	0.61
3:C:63:ALA:HA	3:C:94:HIS:HA	1.82	0.61
1:A:1204:LYS:O	1:A:1204:LYS:HG2	2.01	0.61
1:A:1024:ARG:HA	1:A:1027:ARG:HD3	1.82	0.61
2:D:153:ALA:O	2:D:155:PHE:N	2.34	0.61
1:A:147:PHE:HB3	1:A:151:ASP:HB3	1.83	0.60
1:A:608:THR:HG22	1:A:609:LYS:H	1.67	0.60
1:A:199:ASP:OD2	1:A:246:ARG:NH1	2.35	0.60
2:D:826:THR:OG1	2:D:843:ARG:NH2	2.31	0.60
1:A:1226:ASN:O	1:A:1228:HIS:N	2.34	0.60
2:D:120:ASN:HD21	5:E:1:NAG:H61	1.66	0.60
1:A:546:TYR:OH	1:A:1151:ASP:OD1	2.20	0.60
4:B:5:ILE:HA	4:B:38:GLY:HA2	1.84	0.60
2:D:309:GLN:OE1	2:D:311:ASN:ND2	2.35	0.59
1:A:1117:ASP:OD2	4:B:28:ARG:NH1	2.28	0.59
1:A:1258:MET:HB3	9:A:2304:CLR:H213	1.82	0.59
2:D:152:ASP:OD1	2:D:153:ALA:N	2.35	0.59
2:D:295:ASN:ND2	2:D:328:LYS:O	2.34	0.59
2:D:881:SER:OG	2:D:1021:LYS:NZ	2.35	0.59
1:A:1203:ASP:OD2	1:A:1619:ARG:NH2	2.35	0.58
2:D:850:CYS:H	2:D:863:ASN:HD22	1.51	0.58
4:B:56:ASP:N	4:B:56:ASP:OD1	2.36	0.58
1:A:1302:PRO:HB2	11:A:2307:PT5:H24	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:27:ILE:HG23	4:B:47:PRO:HG2	1.84	0.58
1:A:366:THR:HG21	1:A:1459:ARG:HG3	1.86	0.58
3:C:339:GLU:HG3	3:C:341:GLN:H	1.68	0.58
1:A:605:LEU:O	1:A:607:GLU:N	2.36	0.58
3:C:317:VAL:O	3:C:321:ALA:N	2.31	0.58
1:A:200:PHE:O	1:A:204:VAL:HG23	2.03	0.58
1:A:1104:PRO:HG2	2:D:233:ILE:HG21	1.84	0.58
1:A:1418:LEU:HD22	1:A:1514:LEU:HD12	1.85	0.58
1:A:124:LYS:HB2	1:A:125:PRO:HD2	1.84	0.58
2:D:528:GLN:O	2:D:901:GLN:NE2	2.36	0.58
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.86	0.57
2:D:85:ASP:HB3	2:D:500:LEU:HD22	1.86	0.57
2:D:667:CYS:HB3	2:D:697:CYS:HA	1.85	0.57
2:D:680:LEU:O	2:D:684:ASN:ND2	2.38	0.57
1:A:1122:LEU:HG	9:B:101:CLR:H151	1.86	0.57
2:D:681:LEU:HA	2:D:684:ASN:HD21	1.70	0.57
3:C:97:GLU:HB2	3:C:105:ILE:HB	1.87	0.57
3:C:190:TYR:OH	3:C:311:GLN:O	2.23	0.56
2:D:57:LEU:HD12	2:D:715:LEU:HD22	1.87	0.56
3:C:323:ASP:HB3	3:C:327:GLN:HE22	1.71	0.56
3:C:65:ARG:HB2	3:C:174:VAL:HG21	1.88	0.56
2:D:985:ASN:ND2	2:D:987:SER:OG	2.39	0.56
3:C:136:ARG:O	3:C:137:ARG:NH1	2.38	0.56
2:D:686:PHE:HA	2:D:689:ARG:HG2	1.86	0.56
1:A:134:ILE:HD11	1:A:246:ARG:HE	1.71	0.56
7:G:4:NAG:H83	7:G:4:NAG:H3	1.87	0.56
1:A:1137:TRP:CD1	1:A:1138:PRO:HD3	2.42	0.55
2:D:615:THR:OG1	2:D:616:ASP:N	2.39	0.55
1:A:592:ASP:O	1:A:596:VAL:HG23	2.05	0.55
1:A:902:PHE:O	1:A:903:THR:C	2.44	0.55
1:A:1224:PRO:HG3	1:A:1233:TRP:HB3	1.87	0.55
3:C:100:SER:OG	3:C:102:ASP:OD1	2.24	0.55
7:G:3:NAG:H3	7:G:3:NAG:H83	1.88	0.55
1:A:175:PHE:HD2	1:A:176:LEU:HD12	1.72	0.55
1:A:1017:LEU:HA	1:A:1020:LEU:HB2	1.87	0.55
2:D:631:ILE:HB	2:D:704:ARG:HH12	1.72	0.55
3:C:96:LYS:HD2	3:C:97:GLU:HG2	1.89	0.55
2:D:200:ASP:HB2	2:D:203:LEU:HD22	1.89	0.55
1:A:152:SER:OG	1:A:153:ASN:N	2.40	0.55
1:A:304:ILE:HD12	1:A:333:LYS:HD2	1.89	0.54
3:C:180:VAL:HB	3:C:268:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:SER:HB3	1:A:589:ASN:HB2	1.89	0.54
2:D:1043:PRO:HA	2:D:1046:MET:HB2	1.89	0.54
2:D:185:TRP:HA	5:E:1:NAG:H82	1.87	0.54
2:D:625:THR:HG22	2:D:626:TYR:H	1.72	0.54
1:A:1389:SER:O	1:A:1389:SER:OG	2.24	0.54
2:D:668:ASN:OD1	2:D:668:ASN:N	2.37	0.54
3:C:255:GLU:OE2	3:C:255:GLU:N	2.33	0.53
1:A:410:LYS:HG3	1:A:1531:THR:HG22	1.90	0.53
2:D:747:GLU:OE1	2:D:747:GLU:N	2.35	0.53
3:C:185:PRO:HD2	3:C:193:THR:HG22	1.89	0.53
3:C:179:PRO:HB2	3:C:287:PRO:HB3	1.91	0.53
2:D:779:TYR:HB3	2:D:783:SER:HB3	1.91	0.53
1:A:287:LEU:O	1:A:291:MET:HB2	2.08	0.53
1:A:907:LEU:HD11	1:A:1032:ALA:HB2	1.89	0.53
2:D:716:VAL:HA	2:D:720:TRP:HB2	1.91	0.52
3:C:193:THR:HA	3:C:196:MET:HB2	1.91	0.52
3:C:291:PHE:HB3	3:C:336:ILE:HG23	1.90	0.52
1:A:437:TYR:HB3	3:C:303:LEU:HD21	1.92	0.52
2:D:851:VAL:HG12	2:D:862:ALA:HA	1.90	0.52
2:D:1061:ASP:OD1	2:D:1061:ASP:N	2.42	0.52
3:C:174:VAL:HG12	3:C:175:PRO:HD2	1.90	0.52
1:A:232:ASP:HB2	9:A:2305:CLR:H21	1.92	0.52
4:B:6:HIS:NE2	4:B:11:PRO:HD2	2.24	0.52
2:D:207:VAL:HG23	2:D:217:TYR:HB3	1.90	0.52
1:A:1115:LYS:NZ	1:A:1468:ASP:OD1	2.43	0.52
2:D:459:VAL:HG12	2:D:493:SER:HA	1.92	0.52
3:C:341:GLN:HG3	3:C:343:GLU:H	1.75	0.51
2:D:58:VAL:HG13	2:D:800:ILE:HG22	1.92	0.51
1:A:1432:LYS:O	1:A:1479:CYS:HB2	2.11	0.51
2:D:103:GLU:HG2	2:D:192:VAL:HG21	1.92	0.51
3:C:202:ASP:OD1	3:C:206:HIS:NE2	2.43	0.51
3:C:217:VAL:HG23	3:C:271:ALA:HB2	1.90	0.51
4:B:21:THR:O	4:B:40:GLY:N	2.33	0.51
3:C:178:ARG:HG2	3:C:288:ILE:HG13	1.91	0.51
1:A:175:PHE:O	1:A:179:ILE:HG22	2.09	0.51
2:D:64:TYR:HB3	2:D:67:LEU:HG	1.92	0.51
4:B:10:LEU:HG	4:B:11:PRO:HD3	1.93	0.51
1:A:1212:TYR:OH	1:A:1543:ASP:OD1	2.29	0.50
2:D:851:VAL:HG22	2:D:1016:ILE:HD11	1.93	0.50
2:D:852:ILE:HD11	2:D:861:MET:HB2	1.92	0.50
1:A:1294:LYS:HD2	1:A:1295:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ASN:OD1	2:D:55:ASN:N	2.44	0.50
1:A:380:TRP:N	1:A:381:PRO:HD3	2.26	0.50
1:A:1290:LEU:HD22	1:A:1298:TYR:CD2	2.46	0.50
3:C:304:ILE:HA	3:C:307:ARG:HH21	1.77	0.50
1:A:735:ILE:HD12	9:A:2303:CLR:H242	1.94	0.50
1:A:1373:ILE:HG13	1:A:1375:PHE:H	1.76	0.50
4:B:34:ILE:HG21	4:B:37:ARG:HG3	1.93	0.50
1:A:635:ASN:O	1:A:639:ASN:ND2	2.44	0.50
1:A:686:ARG:NH2	1:A:1146:ASP:OD1	2.45	0.50
1:A:1225:LYS:O	1:A:1227:GLN:N	2.44	0.50
1:A:1312:ILE:HA	1:A:1315:ILE:HD12	1.94	0.50
4:B:5:ILE:HG21	4:B:17:CYS:HB2	1.93	0.50
1:A:1254:ILE:HG23	9:A:2304:CLR:H273	1.94	0.49
1:A:177:LYS:HE2	1:A:196:ASN:HB3	1.94	0.49
1:A:232:ASP:O	1:A:234:LYS:N	2.44	0.49
1:A:902:PHE:CE1	1:A:906:ILE:HG13	2.47	0.49
2:D:631:ILE:HB	2:D:704:ARG:NH1	2.27	0.49
1:A:1225:LYS:C	1:A:1227:GLN:H	2.16	0.49
2:D:890:SER:O	2:D:890:SER:OG	2.29	0.49
1:A:300:ASN:HA	1:A:330:THR:HA	1.93	0.49
2:D:736:THR:HG23	2:D:738:GLY:H	1.76	0.49
2:D:780:PHE:HE1	2:D:870:GLN:HA	1.76	0.49
1:A:1189:PHE:HB3	1:A:1524:MET:HG3	1.94	0.49
1:A:1384:LEU:HD12	1:A:1387:LEU:HD13	1.95	0.49
1:A:1008:SER:OG	1:A:1009:SER:N	2.45	0.49
2:D:1045:ASP:OD1	2:D:1045:ASP:N	2.38	0.49
2:D:659:THR:OG1	2:D:742:ARG:NH1	2.46	0.49
3:C:263:SER:HB2	3:C:265:GLN:HG2	1.95	0.49
3:C:292:VAL:HG12	3:C:337:LEU:HD23	1.94	0.49
1:A:1147:SER:O	1:A:1159:ARG:HD3	2.12	0.49
2:D:736:THR:HG23	2:D:738:GLY:N	2.28	0.49
2:D:773:TYR:HB2	2:D:1011:THR:HG22	1.94	0.49
1:A:443:GLN:O	1:A:447:ILE:HG12	2.12	0.49
1:A:682:MET:HE3	1:A:1099:GLY:HA3	1.95	0.49
1:A:1290:LEU:HD22	1:A:1298:TYR:HE2	1.75	0.48
2:D:985:ASN:OD1	2:D:985:ASN:N	2.46	0.48
1:A:126:PHE:O	1:A:130:ILE:HG12	2.13	0.48
4:B:5:ILE:HG13	4:B:15:LYS:H	1.78	0.48
1:A:994:LEU:O	1:A:998:SER:OG	2.26	0.48
3:C:58:LYS:NZ	3:C:97:GLU:OE2	2.41	0.48
3:C:299:VAL:O	3:C:303:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:22:CYS:HB2	4:B:59:ASN:HD21	1.79	0.48
1:A:1226:ASN:C	1:A:1228:HIS:N	2.67	0.48
1:A:515:ARG:HD2	1:A:516:LYS:HG3	1.94	0.48
1:A:961:THR:O	1:A:965:THR:OG1	2.27	0.48
1:A:1224:PRO:HG2	1:A:1230:TYR:HD1	1.78	0.48
3:C:129:LEU:HD11	3:C:159:LYS:HA	1.96	0.47
1:A:360:ILE:O	1:A:393:SER:OG	2.31	0.47
1:A:158:ASN:O	1:A:162:VAL:HG23	2.14	0.47
1:A:904:ASN:O	1:A:905:LEU:C	2.51	0.47
1:A:1218:PRO:HG3	1:A:1549:TRP:HE1	1.79	0.47
1:A:895:ARG:HG3	1:A:974:ALA:HB2	1.96	0.47
1:A:1224:PRO:HG3	1:A:1233:TRP:CB	2.44	0.47
2:D:747:GLU:H	2:D:747:GLU:CD	2.16	0.47
2:D:806:LEU:O	2:D:807:LEU:HD23	2.14	0.47
1:A:151:ASP:OD1	1:A:152:SER:N	2.47	0.47
1:A:1289:LYS:HB3	1:A:1289:LYS:HE3	1.60	0.47
2:D:594:SER:OG	2:D:596:ASP:O	2.31	0.47
2:D:204:LEU:HD13	2:D:456:LEU:HD21	1.96	0.47
2:D:625:THR:HG22	2:D:626:TYR:N	2.28	0.47
4:B:24:LYS:HB2	4:B:24:LYS:HE3	1.55	0.47
1:A:703:LEU:HD22	1:A:740:GLY:HA3	1.97	0.47
2:D:73:ASN:N	2:D:628:PHE:O	2.47	0.47
2:D:173:TYR:O	2:D:176:SER:OG	2.33	0.47
1:A:519:ALA:O	1:A:523:SER:HB3	2.15	0.47
1:A:1285:GLU:O	1:A:1289:LYS:HG3	2.15	0.46
9:B:101:CLR:H162	9:B:101:CLR:H221	1.65	0.46
1:A:605:LEU:C	1:A:607:GLU:H	2.19	0.46
1:A:622:VAL:O	1:A:625:LEU:HB2	2.15	0.46
1:A:925:HIS:H	1:A:925:HIS:CD2	2.34	0.46
1:A:1221:ARG:HD2	1:A:1221:ARG:HA	1.69	0.46
2:D:744:TYR:HB3	2:D:745:PRO:HD3	1.96	0.46
3:C:216:ARG:NH1	3:C:218:THR:OG1	2.48	0.46
1:A:1220:ARG:NH1	1:A:1554:PRO:O	2.47	0.46
1:A:1298:TYR:CE1	1:A:1304:ASN:HB3	2.50	0.46
2:D:115:GLU:OE2	7:G:3:NAG:O3	2.34	0.46
2:D:990:PHE:O	2:D:1005:GLY:N	2.37	0.46
4:B:22:CYS:HB2	4:B:59:ASN:ND2	2.30	0.46
2:D:88:LYS:HD2	10:D:1202:NAG:H61	1.97	0.46
1:A:597:CYS:SG	1:A:598:GLY:N	2.88	0.46
1:A:996:VAL:HG11	1:A:1027:ARG:HH11	1.81	0.46
1:A:1618:LEU:HD12	1:A:1619:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HD21	1:A:1028:ALA:HA	1.97	0.46
1:A:1605:MET:SD	1:A:1606:PHE:N	2.89	0.46
1:A:1018:ARG:HG3	1:A:1018:ARG:HH11	1.81	0.46
1:A:168:ILE:O	1:A:172:VAL:HG23	2.15	0.45
1:A:533:LEU:HD21	1:A:566:LEU:HD13	1.98	0.45
1:A:544:GLU:OE1	1:A:1069:GLN:NE2	2.49	0.45
1:A:1200:CYS:O	1:A:1201:GLU:HG2	2.15	0.45
2:D:123:VAL:HG12	2:D:143:GLN:HB2	1.97	0.45
1:A:1236:VAL:CG2	1:A:1289:LYS:HG2	2.35	0.45
1:A:896:ILE:HG12	1:A:970:LEU:HD21	1.99	0.45
1:A:1006:ILE:HD11	1:A:1017:LEU:HD12	1.98	0.45
2:D:171:ASP:OD1	2:D:171:ASP:N	2.50	0.45
2:D:616:ASP:N	2:D:616:ASP:OD1	2.45	0.45
4:B:25:MET:O	4:B:35:SER:N	2.50	0.45
1:A:167:LEU:HD21	1:A:207:LEU:HA	1.98	0.45
1:A:1424:VAL:O	1:A:1428:GLN:HG2	2.17	0.45
1:A:1574:PRO:HG3	1:A:1579:GLY:HA2	1.98	0.45
1:A:1394:ILE:HD13	1:A:1394:ILE:HA	1.68	0.45
1:A:177:LYS:HE2	1:A:196:ASN:HD22	1.82	0.45
2:D:688:ASP:N	2:D:688:ASP:OD1	2.41	0.45
2:D:746:LYS:HE3	2:D:746:LYS:HB3	1.66	0.45
3:C:334:ASP:OD1	3:C:334:ASP:N	2.50	0.45
1:A:146:PRO:HG2	1:A:670:MET:HG2	1.99	0.45
1:A:1565:VAL:HA	1:A:1568:LEU:HB3	1.98	0.45
2:D:59:ASP:O	2:D:63:LYS:N	2.49	0.45
1:A:621:CYS:O	1:A:624:LEU:HG	2.16	0.45
2:D:64:TYR:HD1	2:D:711:PHE:HE1	1.65	0.45
3:C:303:LEU:O	3:C:306:SER:OG	2.29	0.45
1:A:773:LYS:HE2	1:A:773:LYS:HB3	1.72	0.44
1:A:1072:LYS:HB3	1:A:1072:LYS:HE3	1.73	0.44
1:A:307:VAL:HG23	1:A:307:VAL:O	2.16	0.44
1:A:1422:TYR:O	1:A:1503:TYR:OH	2.24	0.44
2:D:704:ARG:HD2	2:D:704:ARG:HA	1.68	0.44
1:A:1628:GLN:O	1:A:1631:GLU:HG3	2.17	0.44
2:D:1057:ASP:OD1	2:D:1057:ASP:N	2.34	0.44
3:C:297:PRO:HA	3:C:300:LEU:HD12	1.99	0.44
1:A:380:TRP:H	1:A:381:PRO:HD3	1.83	0.44
1:A:1168:ILE:HG23	1:A:1172:ILE:HD12	2.00	0.44
1:A:1209:CYS:HB3	1:A:1614:VAL:HG11	1.99	0.44
1:A:1291:ILE:O	1:A:1292:ALA:C	2.55	0.44
6:F:2:NAG:O7	6:F:2:NAG:O4	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD11	1:A:403:VAL:HG21	1.98	0.44
2:D:803:GLN:HB2	2:D:805:LYS:HE3	1.99	0.44
4:B:59:ASN:OD1	4:B:59:ASN:N	2.48	0.44
1:A:440:TRP:HA	3:C:342:LEU:HD12	2.00	0.44
2:D:363:ASP:OD1	2:D:363:ASP:N	2.49	0.44
2:D:623:LEU:HD12	2:D:623:LEU:HA	1.87	0.44
1:A:175:PHE:CD2	1:A:176:LEU:HD12	2.52	0.44
1:A:895:ARG:HA	1:A:895:ARG:HD3	1.73	0.44
1:A:927:SER:O	1:A:931:HIS:ND1	2.51	0.44
2:D:79:VAL:HG12	2:D:610:THR:HG22	1.99	0.44
2:D:99:ARG:NH2	2:D:199:GLU:OE2	2.47	0.44
1:A:1221:ARG:HB3	1:A:1223:ILE:HD11	1.99	0.43
2:D:848:MET:HB2	2:D:1019:GLU:HA	2.00	0.43
3:C:204:LEU:HD22	3:C:212:ILE:HG12	1.99	0.43
3:C:255:GLU:HA	3:C:258:PHE:HB2	2.00	0.43
3:C:280:LEU:HD13	3:C:283:THR:HG21	2.01	0.43
1:A:439:ASP:O	1:A:443:GLN:HG2	2.19	0.43
1:A:904:ASN:O	1:A:906:ILE:N	2.52	0.43
2:D:44:LEU:HD11	2:D:821:TRP:HE1	1.83	0.43
1:A:1587:ALA:O	1:A:1590:ARG:HG3	2.18	0.43
4:B:15:LYS:HE2	4:B:16:THR:HG22	2.00	0.43
1:A:434:LEU:HD11	3:C:302:ARG:NE	2.33	0.43
1:A:365:TRP:NE1	1:A:1462:THR:HG21	2.28	0.43
1:A:766:GLN:O	1:A:769:GLU:HG3	2.18	0.43
1:A:1245:MET:O	1:A:1249:ILE:HG13	2.19	0.43
1:A:1619:ARG:HA	1:A:1619:ARG:HD3	1.86	0.43
1:A:1074:LYS:HB3	1:A:1147:SER:HB2	2.01	0.43
1:A:517:CYS:O	1:A:521:VAL:HG23	2.19	0.43
9:A:2304:CLR:H25	9:A:2304:CLR:H222	1.83	0.43
3:C:179:PRO:O	3:C:288:ILE:N	2.40	0.43
3:C:305:ARG:HE	3:C:305:ARG:HB2	1.63	0.43
1:A:199:ASP:OD2	1:A:246:ARG:HD2	2.19	0.43
1:A:362:MET:HG2	1:A:1462:THR:HG23	2.01	0.43
1:A:692:PHE:HB3	1:A:693:PRO:HD3	2.00	0.43
2:D:407:LYS:H	2:D:407:LYS:HG3	1.63	0.43
2:D:537:PRO:HD3	2:D:974:CYS:HB3	2.01	0.43
3:C:92:PHE:HB3	3:C:94:HIS:CE1	2.53	0.43
1:A:175:PHE:CD2	1:A:175:PHE:C	2.93	0.42
1:A:434:LEU:HD21	3:C:302:ARG:HE	1.84	0.42
2:D:401:TRP:CZ2	2:D:405:GLU:HG3	2.54	0.42
2:D:461:THR:HG22	2:D:462:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:771:ASP:OD2	2:D:771:ASP:N	2.35	0.42
2:D:884:ARG:NH2	2:D:1029:ARG:O	2.52	0.42
3:C:64:VAL:N	3:C:93:LEU:O	2.46	0.42
1:A:412:ARG:HG2	1:A:412:ARG:HH11	1.85	0.42
1:A:449:PRO:HB3	3:C:198:LYS:NZ	2.35	0.42
1:A:510:ASN:HA	1:A:513:CYS:HB3	2.01	0.42
1:A:1273:ILE:HG13	1:A:1274:LEU:N	2.33	0.42
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.55	0.42
2:D:157:ARG:NH2	2:D:222:PRO:O	2.52	0.42
2:D:287:ASP:OD1	2:D:287:ASP:N	2.52	0.42
1:A:1399:TRP:CZ2	1:A:1403:LYS:HE2	2.53	0.42
1:A:1049:ILE:HD12	1:A:1181:PHE:HE1	1.84	0.42
1:A:1068:VAL:O	1:A:1072:LYS:HB2	2.20	0.42
2:D:433:PRO:HG2	2:D:1061:ASP:HA	2.01	0.42
1:A:327:GLN:O	1:A:330:THR:OG1	2.37	0.42
1:A:929:ARG:HH12	9:A:2302:CLR:H22	1.84	0.42
2:D:159:ILE:HG22	2:D:221:SER:OG	2.20	0.42
2:D:770:ASN:N	2:D:770:ASN:OD1	2.53	0.42
1:A:773:LYS:O	1:A:776:LYS:HG3	2.20	0.42
1:A:917:LEU:HB2	1:A:1021:ARG:HH21	1.85	0.42
2:D:289:VAL:HG12	2:D:310:ALA:HB2	2.02	0.42
2:D:466:VAL:HG12	2:D:485:LEU:HD12	2.01	0.42
3:C:226:ARG:HD2	3:C:226:ARG:HA	1.77	0.42
1:A:126:PHE:HZ	1:A:173:GLU:HG2	1.84	0.41
1:A:649:ARG:HA	1:A:649:ARG:HD3	1.87	0.41
2:D:440:LYS:NZ	2:D:440:LYS:HB3	2.35	0.41
2:D:449:VAL:HG12	2:D:458:LEU:HD22	2.00	0.41
1:A:137:ASN:OD1	1:A:243:ARG:HD3	2.20	0.41
3:C:178:ARG:NH2	3:C:334:ASP:OD2	2.53	0.41
1:A:912:LEU:HD12	1:A:912:LEU:HA	1.83	0.41
3:C:301:GLN:HG2	3:C:305:ARG:HD3	2.01	0.41
1:A:655:LEU:HD23	1:A:655:LEU:HA	1.93	0.41
1:A:1574:PRO:HB2	1:A:1575:PRO:HD3	2.02	0.41
1:A:1222:TYR:CD1	1:A:1222:TYR:C	2.94	0.41
1:A:1208:GLN:O	1:A:1211:GLU:HG2	2.20	0.41
1:A:1229:GLN:NE2	1:A:1292:ALA:O	2.52	0.41
1:A:1569:LEU:HD11	1:A:1583:PRO:HB3	2.01	0.41
2:D:658:TYR:HB3	2:D:743:VAL:HG13	2.03	0.41
2:D:54:VAL:HG23	2:D:798:VAL:HG12	2.02	0.41
2:D:241:ARG:HA	2:D:241:ARG:HD2	1.94	0.41
2:D:253:ASP:N	2:D:355:ASN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:853:LEU:HD11	2:D:875:PHE:CD1	2.55	0.41
2:D:853:LEU:HD23	2:D:859:LEU:HA	2.03	0.41
2:D:894:PHE:HE2	2:D:896:LYS:HD2	1.85	0.41
2:D:896:LYS:HG2	2:D:979:THR:HG23	2.03	0.41
4:B:19:GLU:HG3	4:B:20:ASN:N	2.36	0.41
1:A:1185:VAL:HG12	1:A:1520:VAL:HG11	2.02	0.41
1:A:1532:ARG:HA	1:A:1532:ARG:HD3	1.96	0.41
3:C:180:VAL:HG22	3:C:288:ILE:HD12	2.03	0.41
1:A:729:VAL:HA	9:A:2303:CLR:H182	2.02	0.41
1:A:1202:LEU:HD12	1:A:1207:ARG:HG3	2.02	0.41
1:A:1287:ILE:O	1:A:1291:ILE:HG13	2.20	0.41
1:A:1467:GLN:H	1:A:1467:GLN:HG3	1.38	0.41
2:D:147:PRO:HG2	2:D:149:PHE:CZ	2.56	0.41
2:D:406:ASN:O	2:D:408:GLY:N	2.50	0.41
2:D:432:ARG:HB2	2:D:433:PRO:HD3	2.03	0.41
2:D:659:THR:HA	2:D:741:THR:O	2.20	0.41
2:D:976:THR:HG22	2:D:1037:THR:HA	2.02	0.41
3:C:220:ASP:O	3:C:221:LEU:HD23	2.20	0.41
3:C:247:ILE:HA	3:C:250:VAL:HG22	2.03	0.41
3:C:358:ARG:HA	3:C:358:ARG:NE	2.36	0.41
1:A:1589:LYS:O	1:A:1593:SER:HB3	2.20	0.41
2:D:1003:PHE:HB3	2:D:1018:VAL:HG23	2.03	0.41
1:A:1589:LYS:HA	1:A:1589:LYS:HD2	1.82	0.40
1:A:1527:PHE:HA	1:A:1530:LEU:HD12	2.03	0.40
2:D:63:LYS:HB2	2:D:63:LYS:HE3	1.86	0.40
2:D:681:LEU:O	2:D:685:GLU:HG2	2.21	0.40
1:A:1049:ILE:HD12	1:A:1181:PHE:CE1	2.56	0.40
1:A:1225:LYS:C	1:A:1227:GLN:N	2.74	0.40
1:A:1298:TYR:CD1	1:A:1304:ASN:HB3	2.56	0.40
1:A:1476:GLY:O	4:B:30:GLN:NE2	2.44	0.40
2:D:704:ARG:NH2	2:D:737:ASP:HB3	2.37	0.40
1:A:307:VAL:O	1:A:309:ALA:N	2.48	0.40
1:A:1101:VAL:HG22	2:D:416:ILE:HD11	2.02	0.40
1:A:1450:PHE:HB3	1:A:1451:PRO:HD3	2.03	0.40
1:A:1640:ILE:HG13	1:A:1642:LYS:H	1.87	0.40
2:D:182:GLU:O	2:D:186:THR:OG1	2.22	0.40
2:D:740:ILE:O	2:D:740:ILE:HD12	2.21	0.40
2:D:881:SER:HG	2:D:1021:LYS:HZ2	1.68	0.40
3:C:102:ASP:OD1	3:C:103:TRP:N	2.54	0.40
3:C:191:GLU:O	3:C:191:GLU:HG2	2.20	0.40
1:A:274:LEU:HD12	1:A:1388:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:PHE:CZ	3:C:178:ARG:HD2	2.57	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	1245/2201 (57%)	1160 (93%)	77 (6%)	8 (1%)	22	52
2	D	936/1103 (85%)	885 (95%)	49 (5%)	2 (0%)	44	73
3	C	322/484 (66%)	302 (94%)	19 (6%)	1 (0%)	37	66
4	B	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
All	All	2561/3848 (67%)	2397 (94%)	153 (6%)	11 (0%)	32	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	1227	GLN
2	D	855	ASP
3	C	331	GLU
1	A	448	ASP
1	A	606	VAL
1	A	610	ILE
1	A	1222	TYR
1	A	1226	ASN
2	D	856	GLY
1	A	1006	ILE

### 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	1118/1896 (59%)	1028 (92%)	90 (8%)	9	29
2	D	837/971 (86%)	777 (93%)	60 (7%)	12	35
3	C	287/426 (67%)	259 (90%)	28 (10%)	6	21
4	B	54/54 (100%)	44 (82%)	10 (18%)	1	4
All	All	2296/3347 (69%)	2108 (92%)	188 (8%)	12	29

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	163	GLU
1	A	164	TYR
1	A	172	VAL
1	A	175	PHE
1	A	177	LYS
1	A	191	LEU
1	A	217	LYS
1	A	231	PHE
1	A	232	ASP
1	A	253	SER
1	A	263	LYS
1	A	302	GLU
1	A	330	THR
1	A	331	VAL
1	A	337	ASP
1	A	348	ASN
1	A	358	GLN
1	A	360	ILE
1	A	426	GLU
1	A	435	LYS
1	A	515	ARG
1	A	518	ARG
1	A	529	LEU

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Mol	Chain	Res	Type
1	A	550	ASN
1	A	554	GLU
1	A	557	ASP
1	A	570	GLU
1	A	574	LYS
1	A	576	TYR
1	A	583	TYR
1	A	584	PHE
1	A	588	PHE
1	A	593	CYS
1	A	597	CYS
1	A	614	LEU
1	A	617	SER
1	A	620	ARG
1	A	632	ARG
1	A	636	SER
1	A	637	LEU
1	A	638	SER
1	A	686	ARG
1	A	691	ASN
1	A	707	ASP
1	A	727	MET
1	A	761	SER
1	A	776	LYS
1	A	898	ASN
1	A	900	THR
1	A	902	PHE
1	A	905	LEU
1	A	907	LEU
1	A	908	PHE
1	A	916	SER
1	A	923	VAL
1	A	931	HIS
1	A	962	SER
1	A	1001	LEU
1	A	1003	SER
1	A	1011	ILE
1	A	1024	ARG
1	A	1042	VAL
1	A	1095	THR
1	A	1126	MET
1	A	1159	ARG

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Mol	Chain	Res	Type
1	A	1192	GLN
1	A	1200	CYS
1	A	1219	LEU
1	A	1221	ARG
1	A	1225	LYS
1	A	1228	HIS
1	A	1271	MET
1	A	1288	LEU
1	A	1290	LEU
1	A	1298	TYR
1	A	1309	LEU
1	A	1376	PHE
1	A	1380	ARG
1	A	1386	LYS
1	A	1389	SER
1	A	1390	ARG
1	A	1394	ILE
1	A	1436	ASN
1	A	1467	GLN
1	A	1483	SER
1	A	1549	TRP
1	A	1564	ASP
1	A	1596	MET
1	A	1605	MET
2	D	31	VAL
2	D	37	VAL
2	D	39	LYS
2	D	40	MET
2	D	52	SER
2	D	59	ASP
2	D	68	TYR
2	D	106	LYS
2	D	114	ARG
2	D	143	GLN
2	D	176	SER
2	D	203	LEU
2	D	246	GLN
2	D	250	SER
2	D	268	THR
2	D	287	ASP
2	D	311	ASN
2	D	338	SER

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Mol	Chain	Res	Type
2	D	407	LYS
2	D	421	ILE
2	D	460	ILE
2	D	476	LYS
2	D	495	GLU
2	D	506	LEU
2	D	507	CYS
2	D	523	LEU
2	D	538	THR
2	D	553	SER
2	D	555	GLU
2	D	591	LEU
2	D	602	LYS
2	D	670	LEU
2	D	673	SER
2	D	682	ASN
2	D	734	VAL
2	D	741	THR
2	D	743	VAL
2	D	745	PRO
2	D	747	GLU
2	D	783	SER
2	D	788	TYR
2	D	798	VAL
2	D	805	LYS
2	D	806	LEU
2	D	816	ILE
2	D	820	SER
2	D	823	GLU
2	D	848	MET
2	D	850	CYS
2	D	866	ASP
2	D	881	SER
2	D	883	MET
2	D	897	SER
2	D	972	GLN
2	D	973	SER
2	D	1009	MET
2	D	1029	ARG
2	D	1037	THR
2	D	1045	ASP
2	D	1071	CYS

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Mol	Chain	Res	Type
3	C	96	LYS
3	C	107	ARG
3	C	109	VAL
3	C	110	LYS
3	C	174	VAL
3	C	186	SER
3	C	203	PHE
3	C	211	ARG
3	C	216	ARG
3	C	256	ARG
3	C	257	ILE
3	C	264	LEU
3	C	267	VAL
3	C	282	LYS
3	C	290	VAL
3	C	293	LYS
3	C	296	SER
3	C	303	LEU
3	C	307	ARG
3	C	312	MET
3	C	315	LEU
3	C	320	MET
3	C	322	TYR
3	C	323	ASP
3	C	325	LEU
3	C	342	LEU
3	C	344	ASP
3	C	361	HIS
4	B	4	TYR
4	B	5	ILE
4	B	14	THR
4	B	22	CYS
4	B	41	CYS
4	B	46	TRP
4	B	49	GLN
4	B	54	LYS
4	B	57	ARG
4	B	59	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	429	GLN
1	A	904	ASN
2	D	684	ASN
2	D	863	ASN
2	D	901	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	$\# Z  > 2$
5	NAG	E	1	2,5	14,14,15	0.58	0	17,19,21	2.03	3 (17%)
5	NAG	E	2	5	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	E	3	5	14,14,15	0.33	0	17,19,21	0.38	0
6	NAG	F	1	2,6	14,14,15	0.49	0	17,19,21	0.82	1 (5%)
6	NAG	F	2	6	14,14,15	0.66	1 (7%)	17,19,21	0.79	0
7	NAG	G	1	7,2	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	G	2	7	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	G	3	7	14,14,15	1.02	1 (7%)	17,19,21	1.66	2 (11%)
7	NAG	G	4	7	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
6	NAG	H	1	2,6	14,14,15	0.27	0	17,19,21	0.43	0
6	NAG	H	2	6	14,14,15	0.30	0	17,19,21	0.45	0
6	NAG	I	1	2,6	14,14,15	0.51	0	17,19,21	0.40	0
6	NAG	I	2	6	14,14,15	0.22	0	17,19,21	0.41	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
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
5	NAG	E	3	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
7	NAG	G	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	NAG	G	3	7	-	5/6/23/26	0/1/1/1
7	NAG	G	4	7	-	5/6/23/26	0/1/1/1
6	NAG	H	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	NAG	I	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	NAG	O5-C1	3.32	1.49	1.43
6	F	2	NAG	O5-C1	-2.29	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	7.25	122.02	112.19
7	G	3	NAG	C1-O5-C5	4.58	118.40	112.19
7	G	3	NAG	C2-N2-C7	4.35	129.10	122.90
7	G	4	NAG	C2-N2-C7	4.29	129.01	122.90
5	E	1	NAG	C3-C4-C5	3.04	115.65	110.24
5	E	1	NAG	O5-C5-C4	2.56	117.06	110.83
6	F	1	NAG	C1-O5-C5	2.52	115.61	112.19

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	3	NAG	O5-C5-C6-O6

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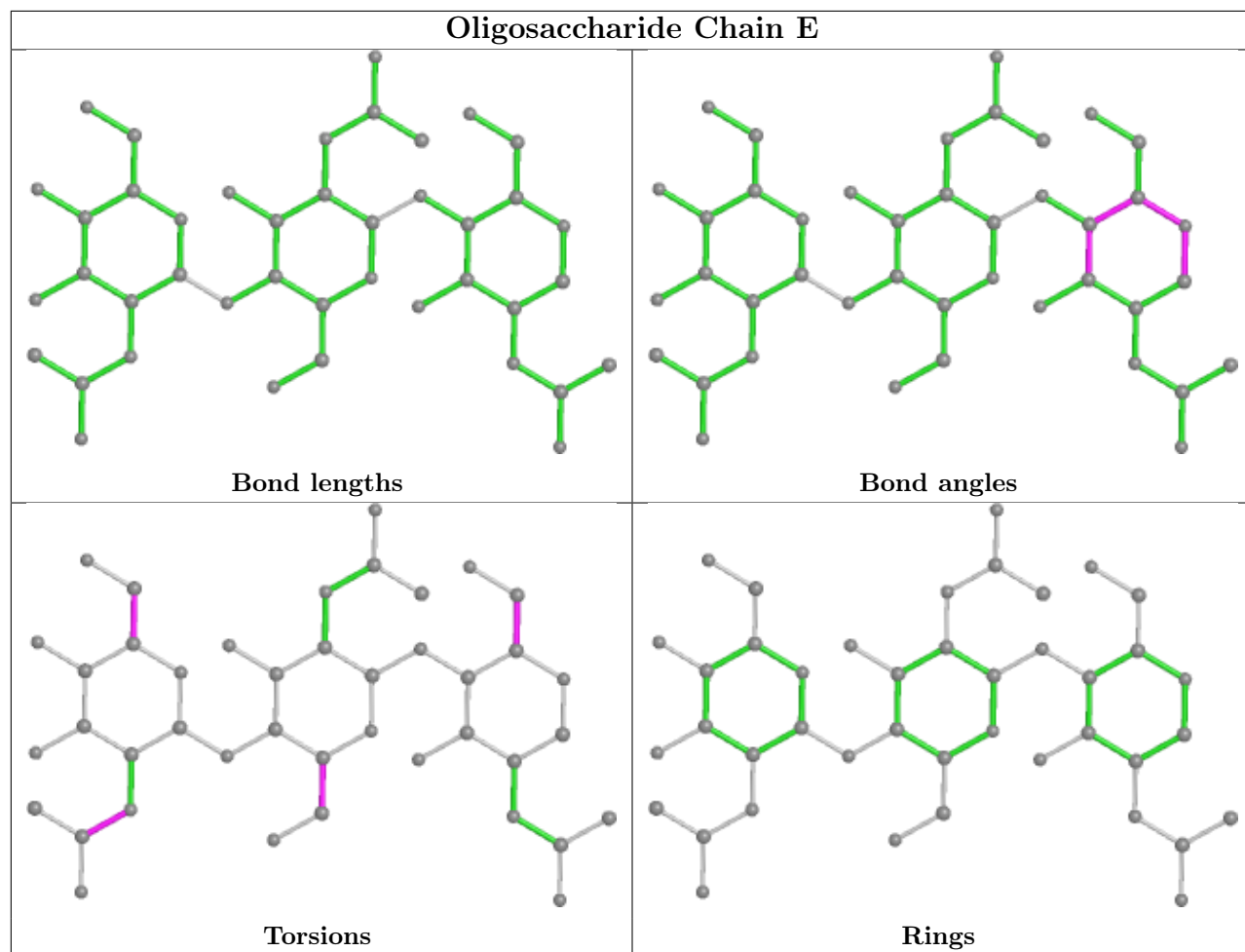
Mol	Chain	Res	Type	Atoms
7	G	3	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
7	G	4	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
7	G	4	NAG	O5-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
5	E	3	NAG	C8-C7-N2-C2
5	E	3	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2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

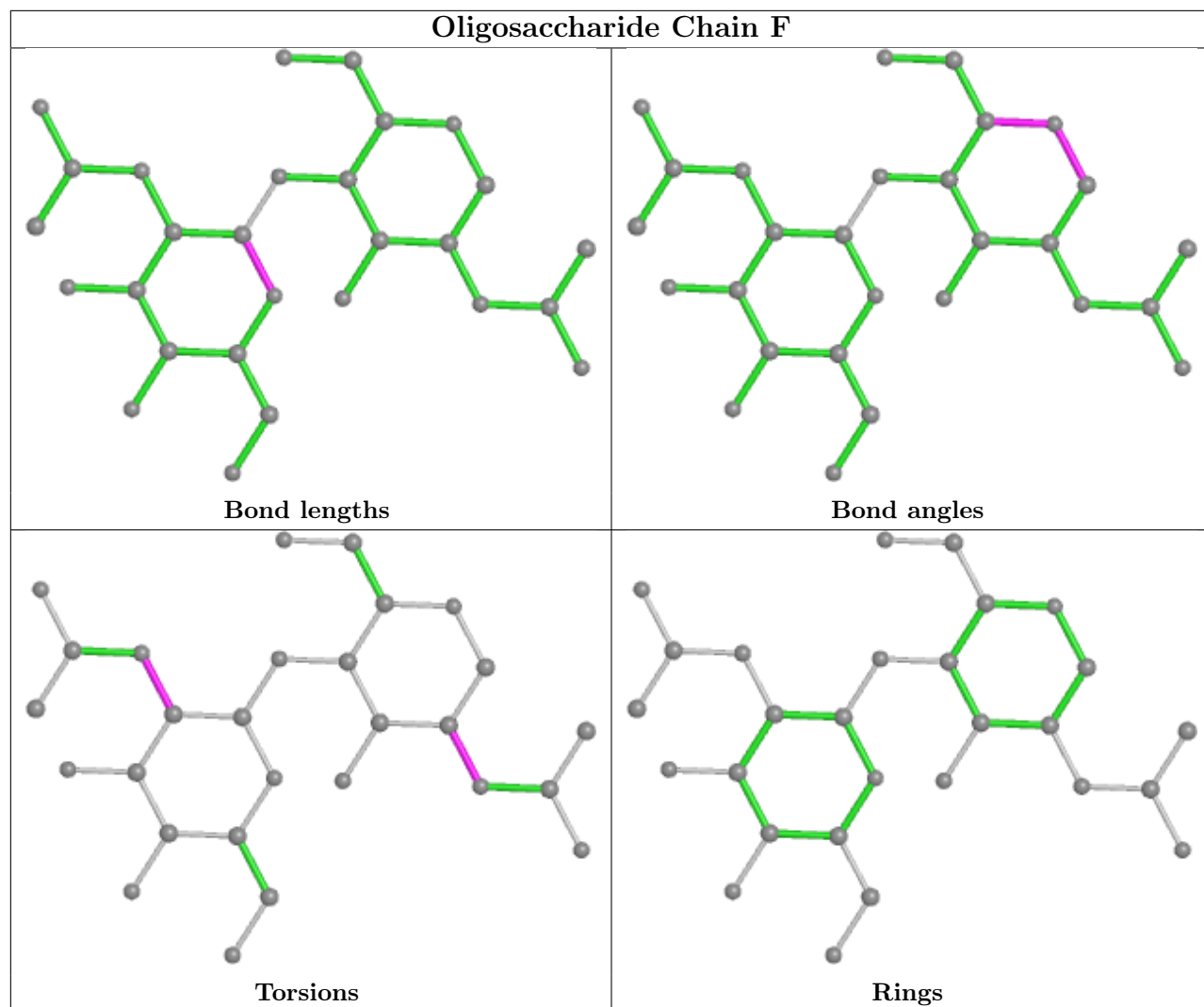
There are no ring outliers.

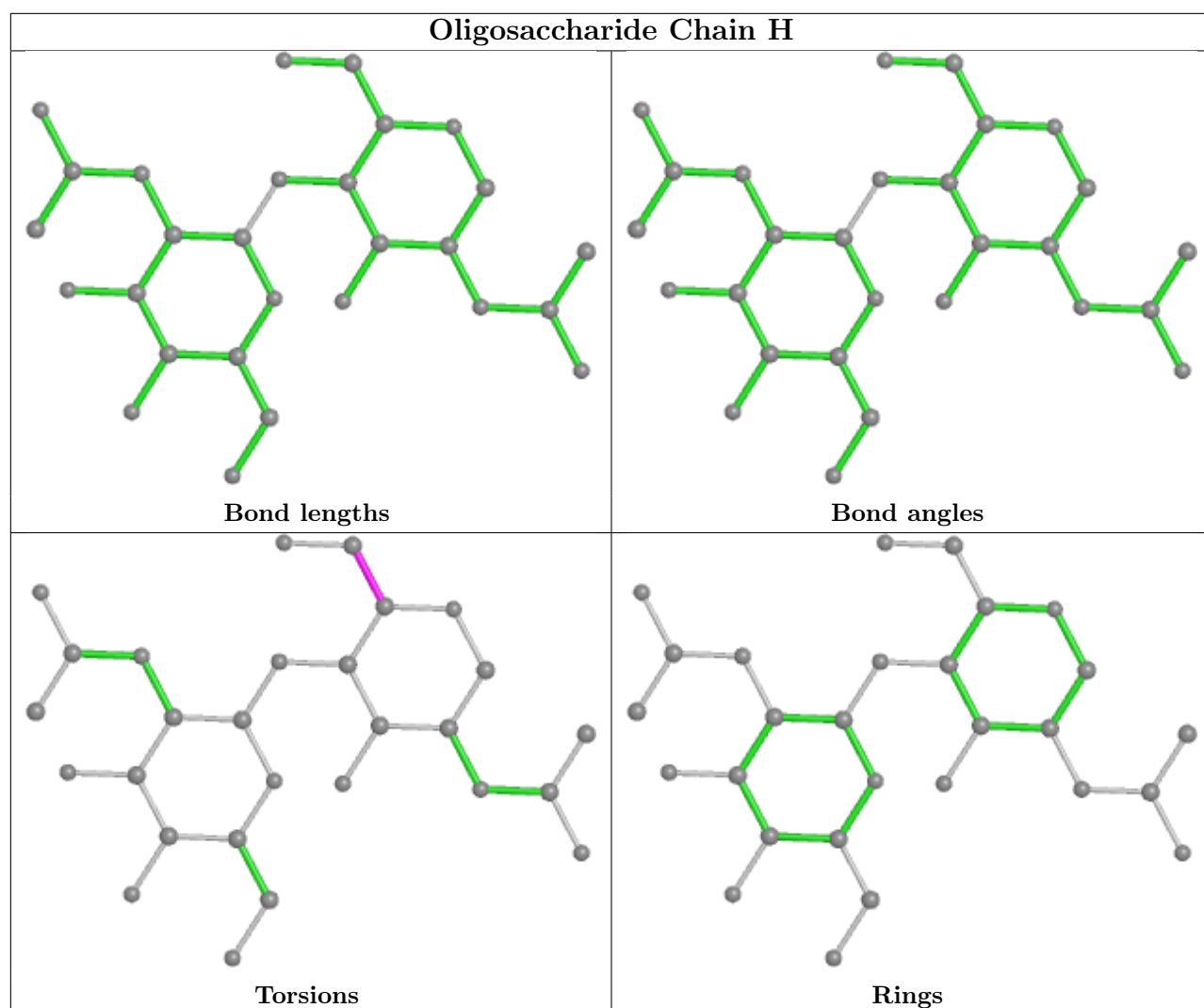
4 monomers are involved in 6 short contacts:

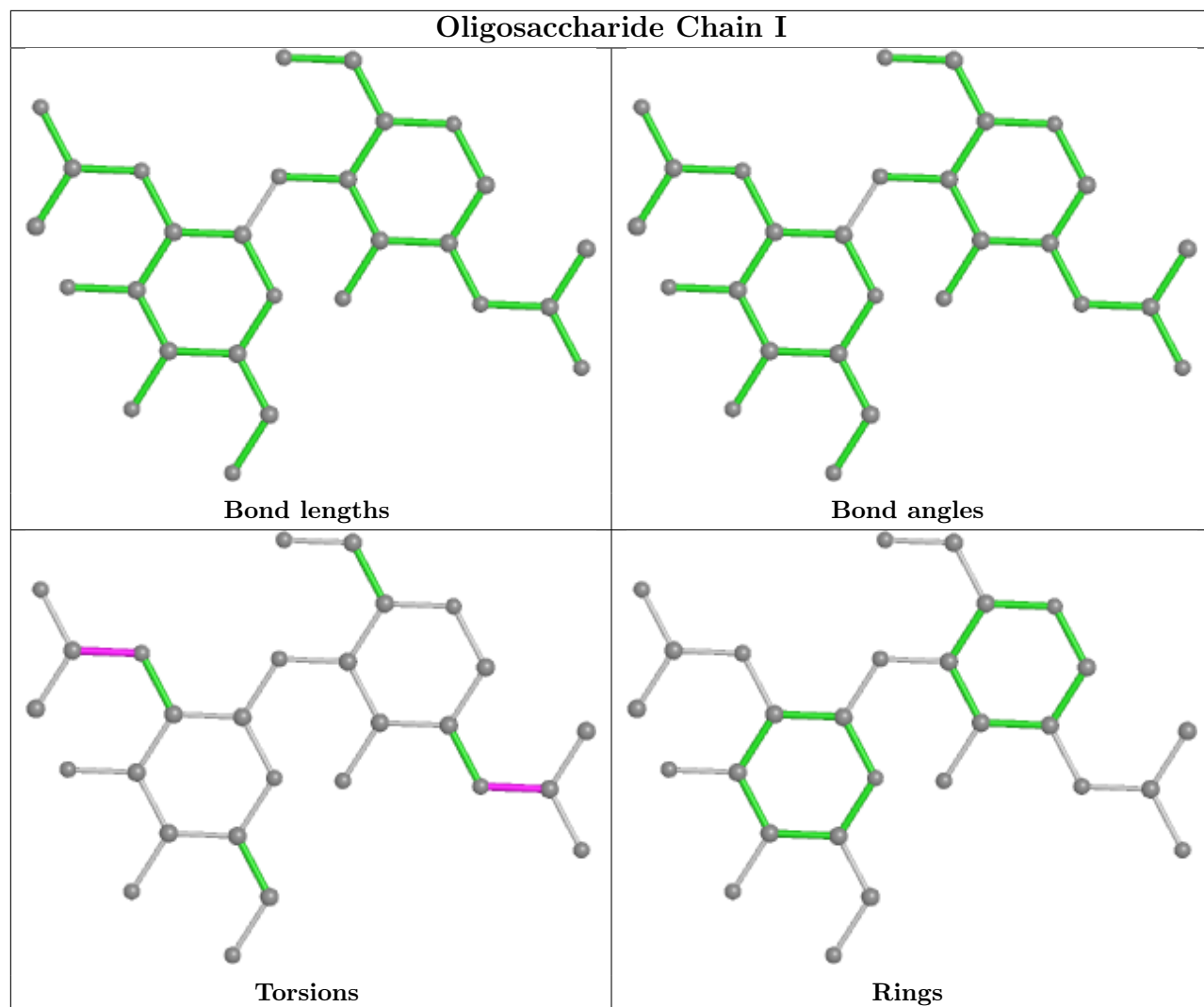
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
6	F	2	NAG	1	0
7	G	4	NAG	1	0
7	G	3	NAG	2	0

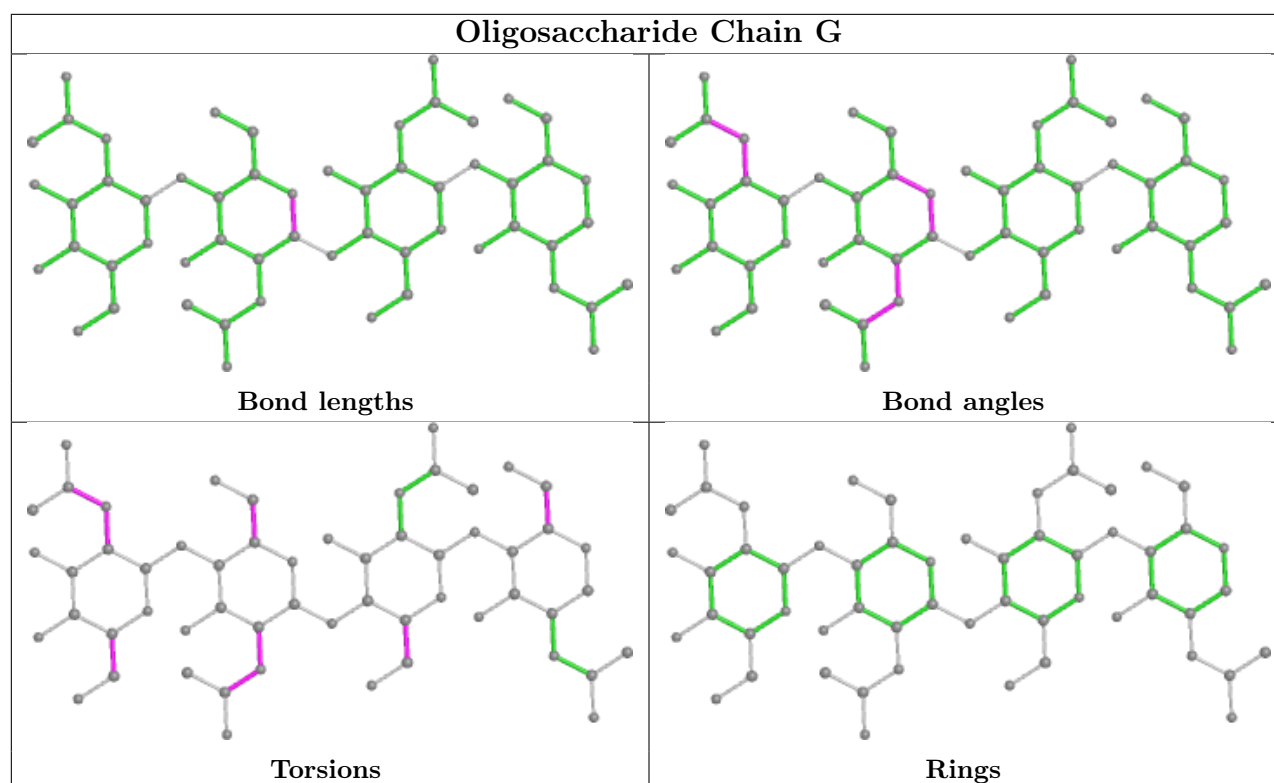
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
10	NAG	A	2306	1	14,14,15	0.29	0	17,19,21	0.41	0
9	CLR	A	2302	-	31,31,31	0.36	0	48,48,48	0.56	0
13	6UB	A	2309	-	29,29,29	2.00	10 (34%)	37,39,39	2.49	14 (37%)
11	PT5	A	2307	-	63,63,69	0.87	2 (3%)	76,81,87	1.03	3 (3%)
12	3PE	A	2308	-	37,37,50	0.58	0	40,42,55	0.60	1 (2%)
9	CLR	B	101	-	31,31,31	0.37	0	48,48,48	0.66	0
9	CLR	A	2303	-	31,31,31	0.37	0	48,48,48	0.53	0
9	CLR	A	2305	-	31,31,31	0.40	0	48,48,48	0.75	1 (2%)
10	NAG	D	1203	2	14,14,15	0.87	1 (7%)	17,19,21	1.03	1 (5%)
10	NAG	D	1202	2	14,14,15	0.33	0	17,19,21	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CLR	A	2304	-	31,31,31	0.39	0	48,48,48	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	2306	1	-	2/6/23/26	0/1/1/1
9	CLR	A	2302	-	-	3/10/68/68	0/4/4/4
13	6UB	A	2309	-	-	15/22/42/42	0/2/2/2
11	PT5	A	2307	-	-	28/60/84/90	0/1/1/1
12	3PE	A	2308	-	-	22/41/41/54	-
9	CLR	B	101	-	-	6/10/68/68	0/4/4/4
9	CLR	A	2303	-	-	5/10/68/68	0/4/4/4
9	CLR	A	2305	-	-	5/10/68/68	0/4/4/4
10	NAG	D	1203	2	-	2/6/23/26	0/1/1/1
10	NAG	D	1202	2	-	1/6/23/26	0/1/1/1
9	CLR	A	2304	-	-	4/10/68/68	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2307	PT5	O18-C11	4.04	1.45	1.33
13	A	2309	6UB	CAT-CAX	-4.04	1.30	1.35
11	A	2307	PT5	O16-C10	3.98	1.45	1.34
13	A	2309	6UB	CAW-NAP	3.87	1.43	1.37
13	A	2309	6UB	CAT-NAP	3.35	1.43	1.38
13	A	2309	6UB	CAV-CAY	3.20	1.53	1.47
13	A	2309	6UB	OAS-CAV	3.13	1.39	1.33
10	D	1203	NAG	O5-C1	2.88	1.48	1.43
13	A	2309	6UB	CAU-CAX	2.56	1.52	1.47
13	A	2309	6UB	OAQ-CAB	-2.51	1.39	1.45
13	A	2309	6UB	OAQ-CAU	2.30	1.38	1.33
13	A	2309	6UB	CBB-CAY	2.12	1.54	1.52
13	A	2309	6UB	CAW-CAY	-2.12	1.33	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	2309	6UB	CAC-CAT-CAX	-7.32	120.30	127.62
13	A	2309	6UB	CBA-CAZ-CLAG	5.85	126.47	120.41
13	A	2309	6UB	OAS-CAV-CAY	4.75	120.78	112.31
10	D	1203	NAG	C1-O5-C5	4.01	117.63	112.19
11	A	2307	PT5	O16-C10-C12	3.97	120.05	111.50
13	A	2309	6UB	OAQ-CAU-CAX	3.76	119.01	112.30
13	A	2309	6UB	CAK-CBA-CBB	-3.37	113.11	119.44
13	A	2309	6UB	CAZ-CBA-CBB	3.29	128.37	123.98
13	A	2309	6UB	CAL-OAS-CAV	-3.28	110.69	116.50
13	A	2309	6UB	OAS-CAV-OAF	-3.19	117.59	123.34
13	A	2309	6UB	CAC-CAT-NAP	3.15	117.19	113.45
11	A	2307	PT5	O18-C11-C31	3.12	121.71	111.91
13	A	2309	6UB	CAX-CBB-CAY	2.68	114.23	109.78
13	A	2309	6UB	CAJ-CAZ-CBA	-2.62	119.61	121.99
11	A	2307	PT5	O18-C11-O19	-2.47	117.35	123.59
13	A	2309	6UB	OAQ-CAU-OAE	-2.47	118.78	123.53
12	A	2308	3PE	O12-P-O14	2.35	123.84	112.24
13	A	2309	6UB	CAJ-CAZ-CLAG	-2.23	113.92	118.41
13	A	2309	6UB	CBB-CAY-CAV	-2.15	111.94	117.15
9	A	2305	CLR	C17-C13-C14	2.01	102.45	100.07

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2307	PT5	C3-C4-O4-P4
11	A	2307	PT5	C6-C5-O5-P5
11	A	2307	PT5	C4-C5-O5-P5
11	A	2307	PT5	C5-O5-P5-O52
11	A	2307	PT5	C16-C17-C18-C19
12	A	2308	3PE	C1-O11-P-O12
12	A	2308	3PE	C11-O13-P-O11
12	A	2308	3PE	C11-O13-P-O12
12	A	2308	3PE	C11-O13-P-O14
13	A	2309	6UB	O25-C24-CAW-CAY
13	A	2309	6UB	O25-C24-CAW-NAP
10	A	2306	NAG	C4-C5-C6-O6
9	B	101	CLR	C21-C20-C22-C23
9	B	101	CLR	C13-C17-C20-C22
13	A	2309	6UB	OAF-CAV-OAS-CAL
13	A	2309	6UB	CAY-CAV-OAS-CAL
13	A	2309	6UB	CAX-CAU-OAQ-CAB
10	A	2306	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	101	CLR	C16-C17-C20-C21
10	D	1203	NAG	C4-C5-C6-O6
12	A	2308	3PE	O22-C21-O21-C2
9	A	2304	CLR	C21-C20-C22-C23
9	B	101	CLR	C13-C17-C20-C21
12	A	2308	3PE	C22-C21-O21-C2
10	D	1203	NAG	O5-C5-C6-O6
9	B	101	CLR	C16-C17-C20-C22
9	A	2302	CLR	C21-C20-C22-C23
12	A	2308	3PE	C32-C31-O31-C3
9	A	2305	CLR	C17-C20-C22-C23
11	A	2307	PT5	O16-C8-C9-O18
13	A	2309	6UB	OAE-CAU-OAQ-CAB
9	A	2304	CLR	C17-C20-C22-C23
9	B	101	CLR	C17-C20-C22-C23
12	A	2308	3PE	O32-C31-O31-C3
12	A	2308	3PE	C1-O11-P-O13
11	A	2307	PT5	C12-C10-O16-C8
12	A	2308	3PE	C39-C3A-C3B-C3C
12	A	2308	3PE	C24-C25-C26-C27
11	A	2307	PT5	O17-C10-O16-C8
11	A	2307	PT5	C33-C34-C35-C36
12	A	2308	3PE	C37-C38-C39-C3A
13	A	2309	6UB	OAE-CAU-CAX-CBB
13	A	2309	6UB	CAW-C24-O25-C26
12	A	2308	3PE	C34-C35-C36-C37
12	A	2308	3PE	C25-C26-C27-C28
13	A	2309	6UB	OAQ-CAU-CAX-CBB
11	A	2307	PT5	C42-C43-C44-C45
9	A	2303	CLR	C20-C22-C23-C24
11	A	2307	PT5	C12-C13-C14-C15
9	A	2305	CLR	C21-C20-C22-C23
11	A	2307	PT5	C31-C11-O18-C9
11	A	2307	PT5	C7-C8-C9-O18
12	A	2308	3PE	C1-C2-C3-O31
9	A	2305	CLR	C22-C23-C24-C25
12	A	2308	3PE	C26-C27-C28-C29
9	A	2304	CLR	C20-C22-C23-C24
11	A	2307	PT5	O19-C11-O18-C9
11	A	2307	PT5	C35-C36-C37-C38
12	A	2308	3PE	O13-C11-C12-N
11	A	2307	PT5	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
11	A	2307	PT5	C7-O13-P1-O1
13	A	2309	6UB	CAZ-CBA-CBB-CAY
13	A	2309	6UB	CAZ-CBA-CBB-CAX
12	A	2308	3PE	O11-C1-C2-O21
12	A	2308	3PE	O21-C2-C3-O31
12	A	2308	3PE	C1-O11-P-O14
11	A	2307	PT5	C10-C12-C13-C14
13	A	2309	6UB	C27-C26-O25-C24
11	A	2307	PT5	C7-C8-O16-C10
10	D	1202	NAG	C3-C2-N2-C7
13	A	2309	6UB	OAE-CAU-CAX-CAT
13	A	2309	6UB	OAQ-CAU-CAX-CAT
11	A	2307	PT5	C18-C19-C20-C21
11	A	2307	PT5	C19-C20-C21-C22
9	A	2303	CLR	C22-C23-C24-C25
9	A	2305	CLR	C23-C24-C25-C26
12	A	2308	3PE	C36-C37-C38-C39
12	A	2308	3PE	C3B-C3C-C3D-C3E
11	A	2307	PT5	O16-C10-C12-C13
9	A	2302	CLR	C13-C17-C20-C21
9	A	2303	CLR	C13-C17-C20-C21
11	A	2307	PT5	C5-C4-O4-P4
11	A	2307	PT5	C4-O4-P4-O41
11	A	2307	PT5	C34-C35-C36-C37
13	A	2309	6UB	CAK-CBA-CBB-CAX
11	A	2307	PT5	C41-C42-C43-C44
9	A	2305	CLR	C23-C24-C25-C27
9	A	2303	CLR	C17-C20-C22-C23
9	A	2304	CLR	C22-C23-C24-C25
9	A	2303	CLR	C16-C17-C20-C22
11	A	2307	PT5	O17-C10-C12-C13
11	A	2307	PT5	C7-O13-P1-O11
9	A	2302	CLR	C16-C17-C20-C22

There are no ring outliers.

7 monomers are involved in 11 short contacts:

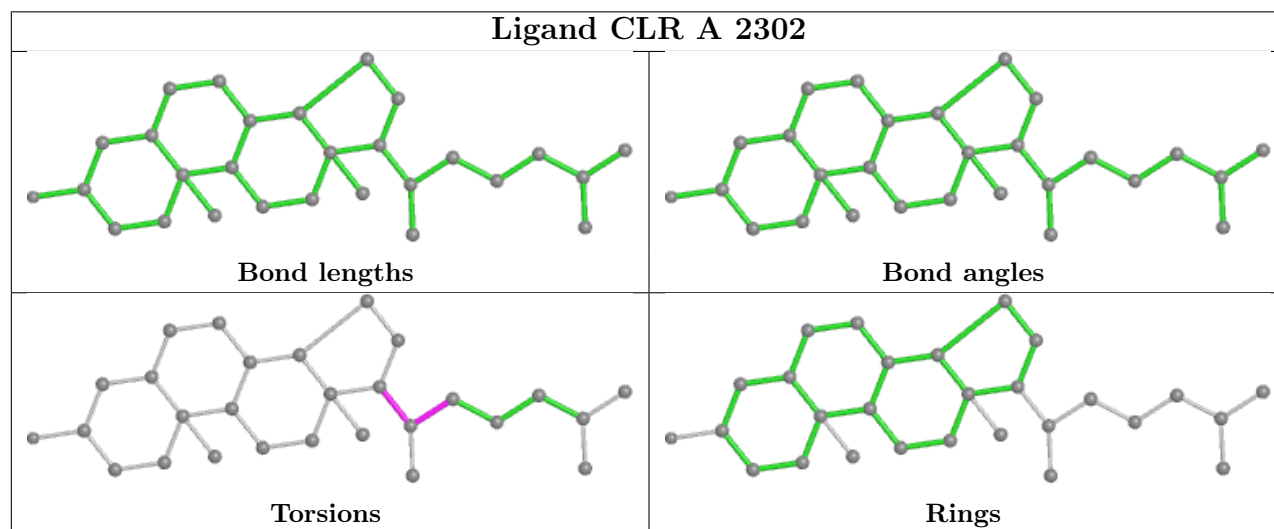
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2302	CLR	1	0
11	A	2307	PT5	1	0
9	B	101	CLR	2	0
9	A	2303	CLR	2	0

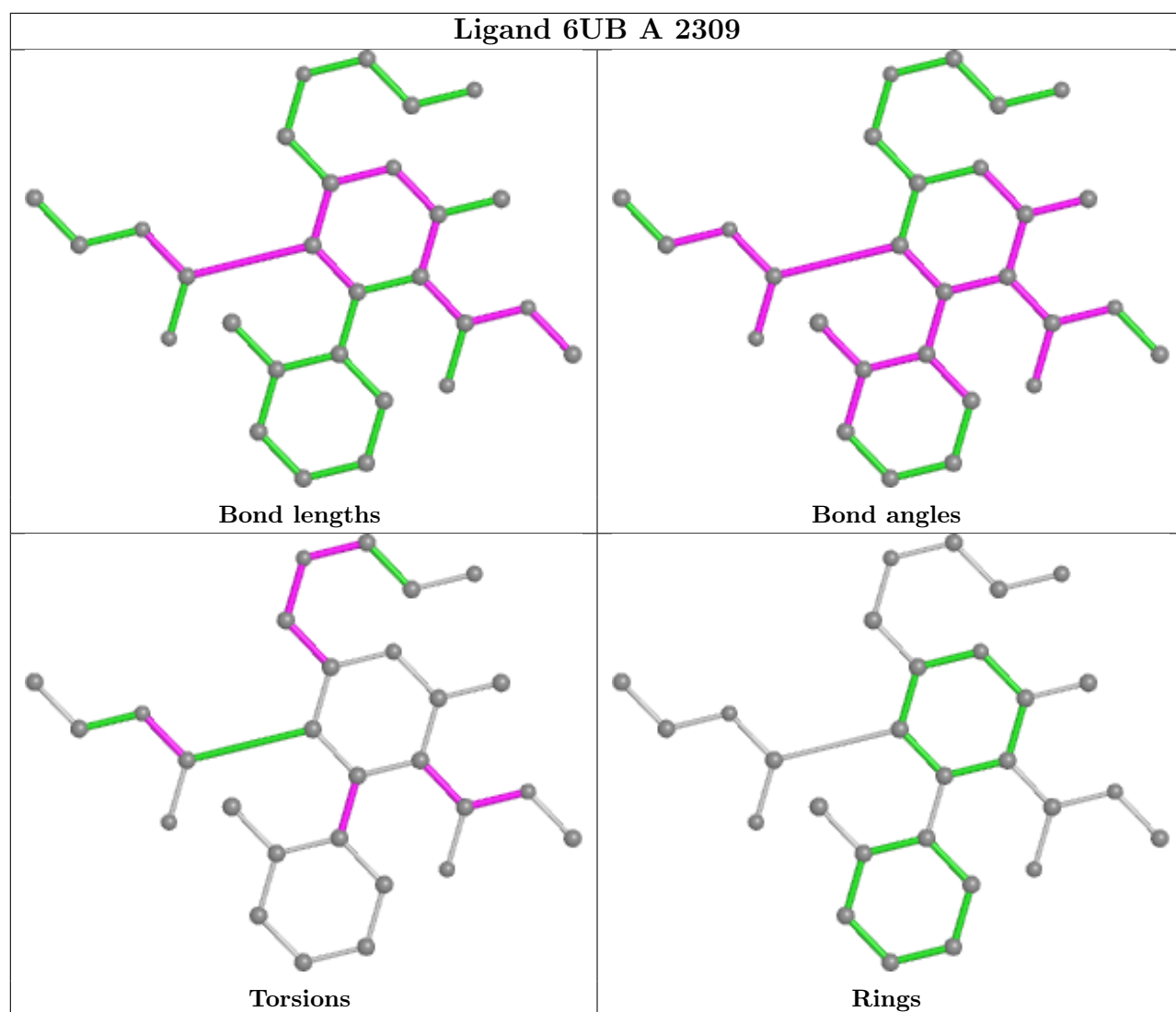
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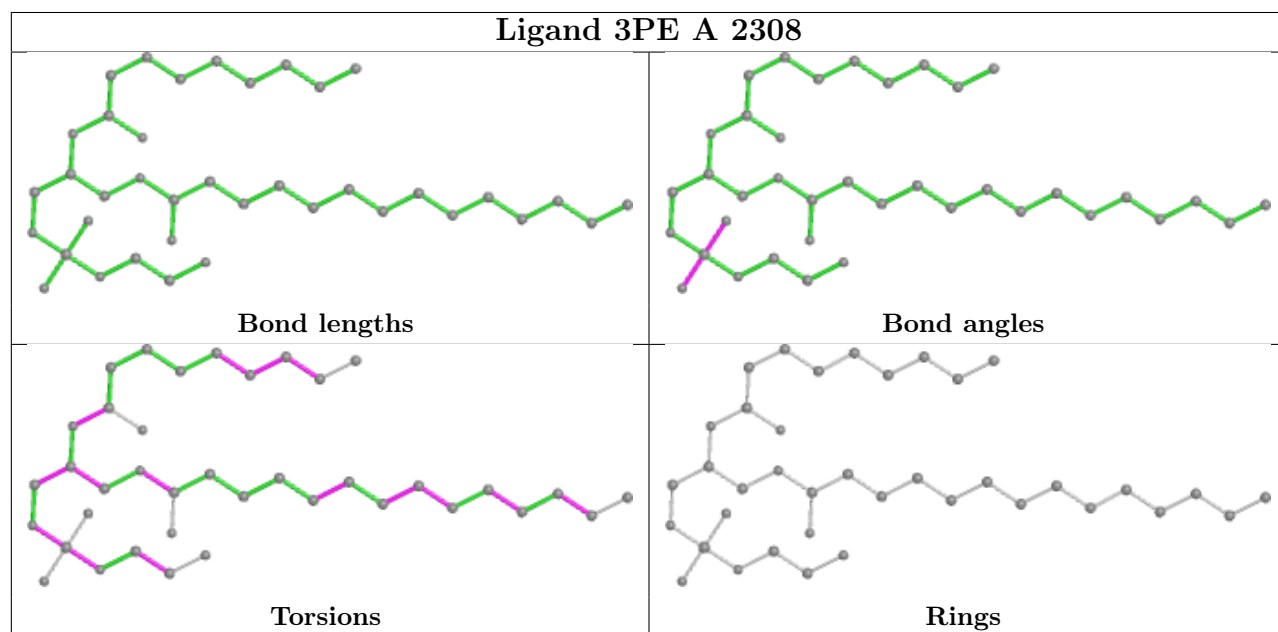
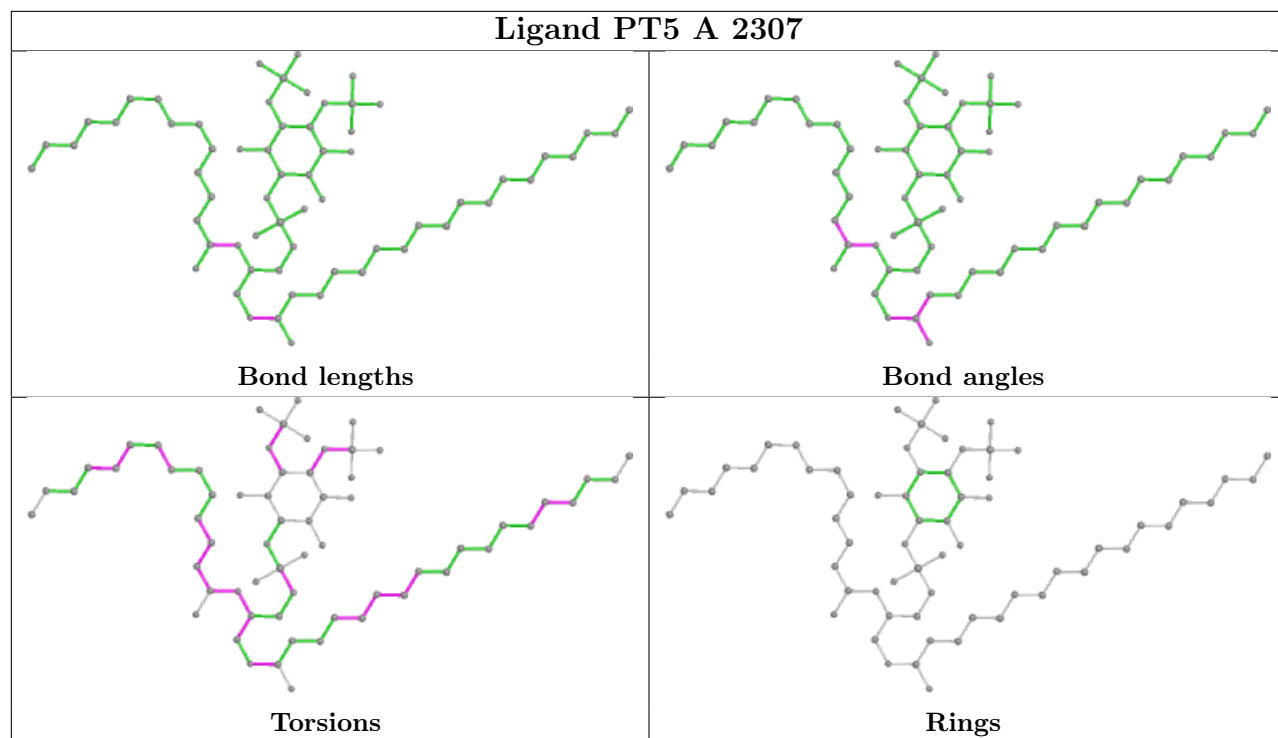
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2305	CLR	1	0
10	D	1202	NAG	1	0
9	A	2304	CLR	3	0

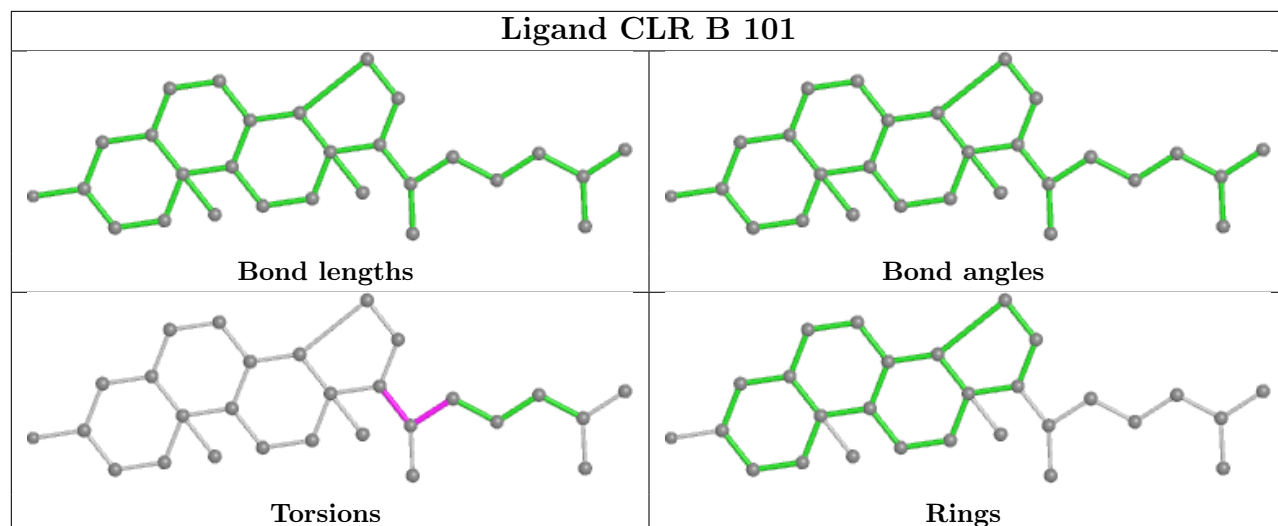
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



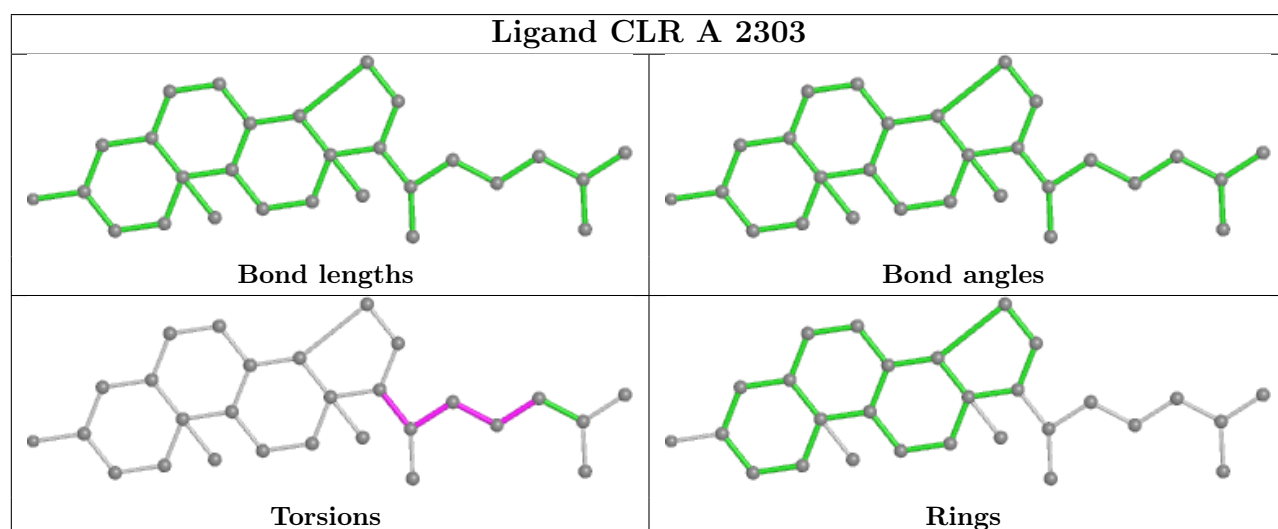




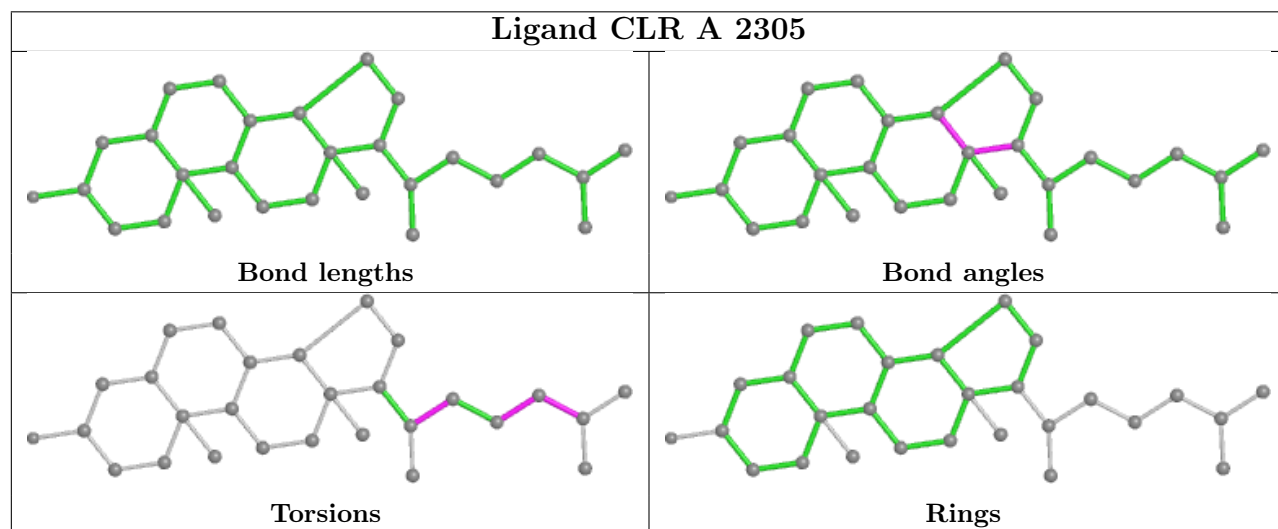
## Ligand CLR B 101



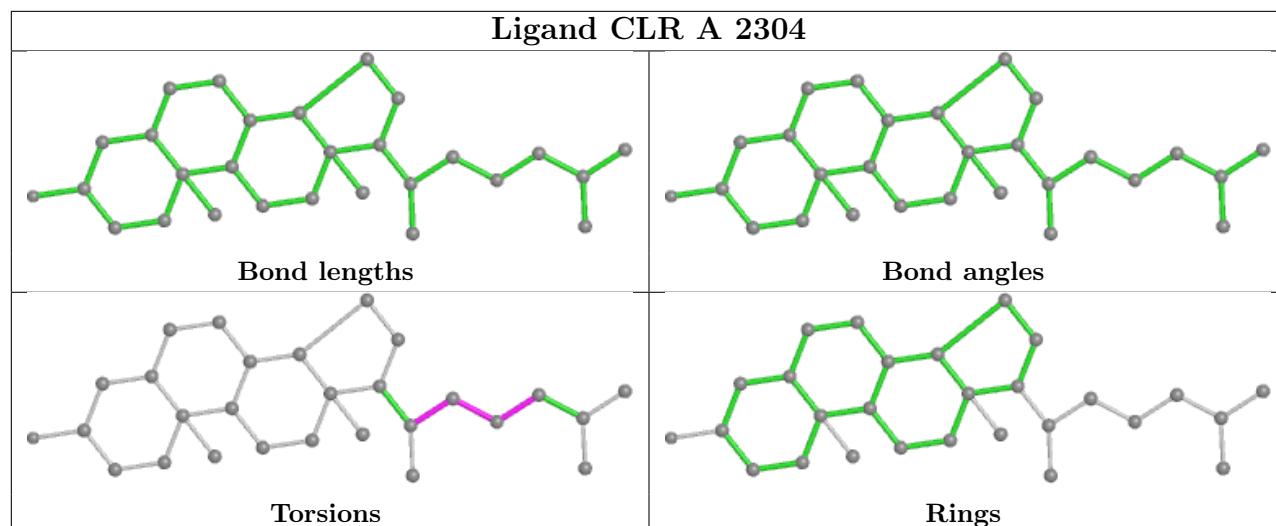
## Ligand CLR A 2303



## Ligand CLR A 2305







## 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.

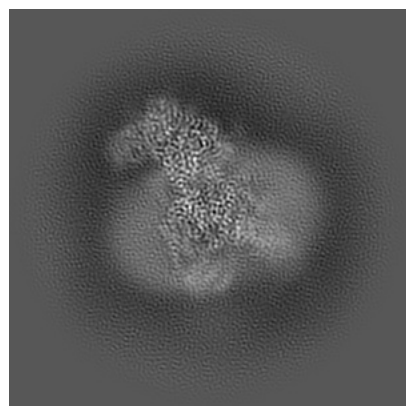
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37474. These allow visual inspection of the internal detail of the map and identification of artifacts.

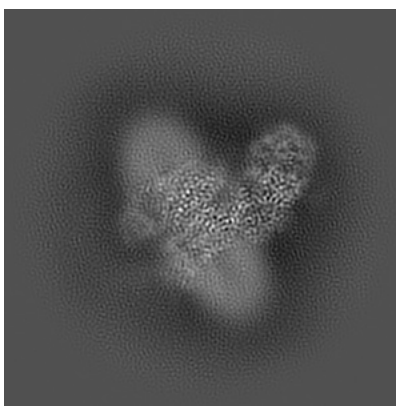
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

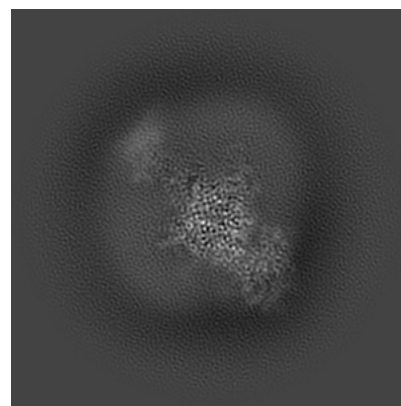
#### 6.1.1 Primary map



X

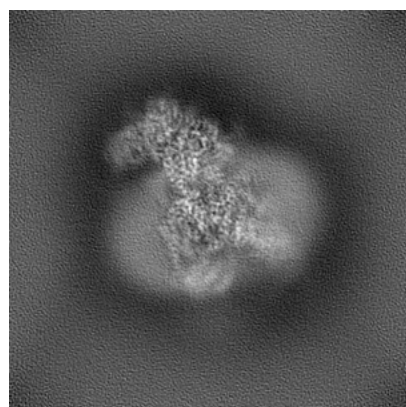


Y

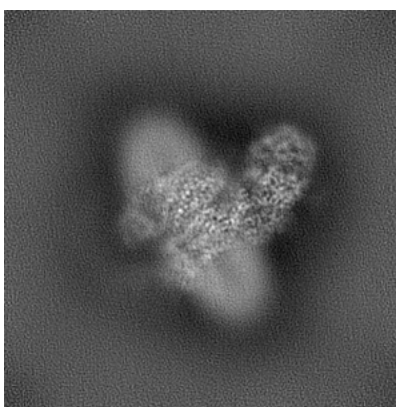


Z

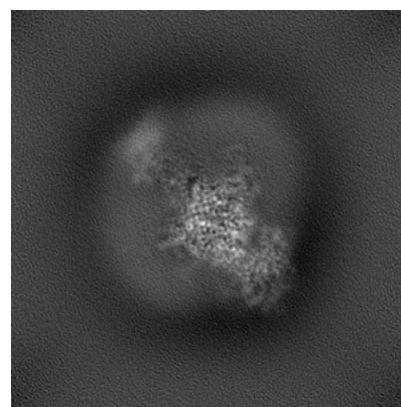
#### 6.1.2 Raw map



X



Y

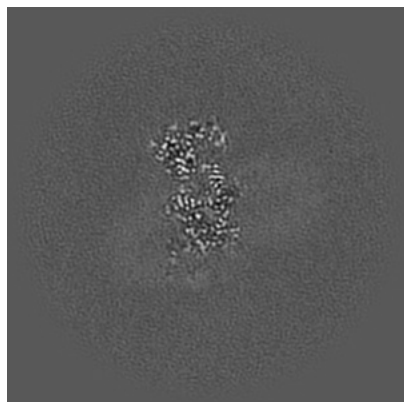


Z

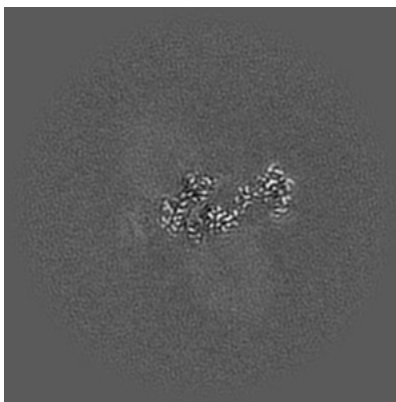
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

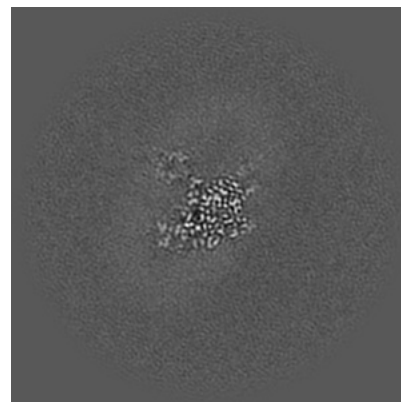
### 6.2.1 Primary map



X Index: 140

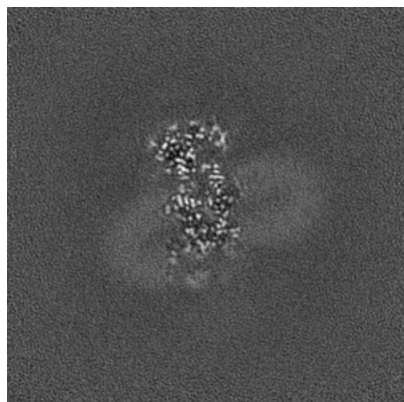


Y Index: 140

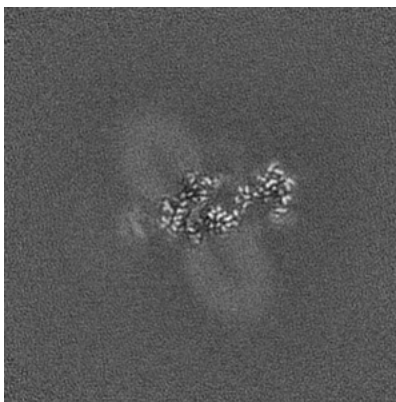


Z Index: 140

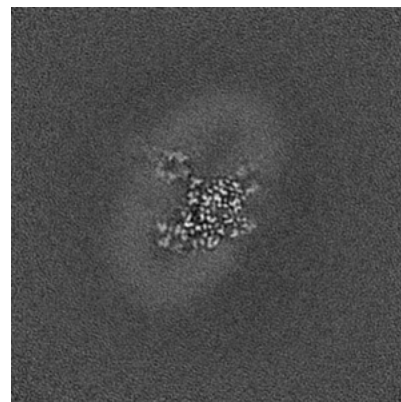
### 6.2.2 Raw map



X Index: 140



Y Index: 140

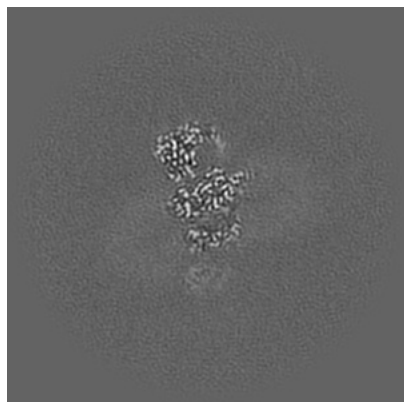


Z Index: 140

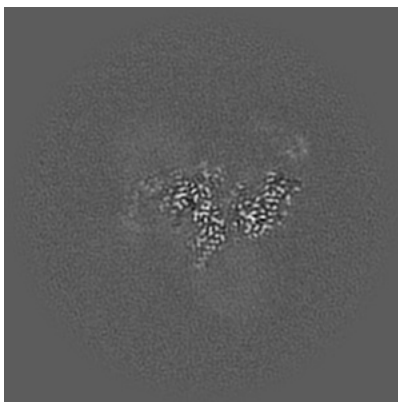
The images above show central slices of the map in three orthogonal directions.

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

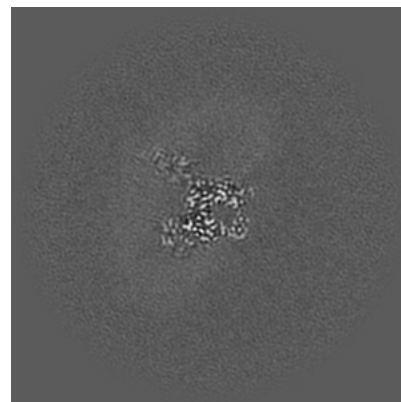
### 6.3.1 Primary map



X Index: 135

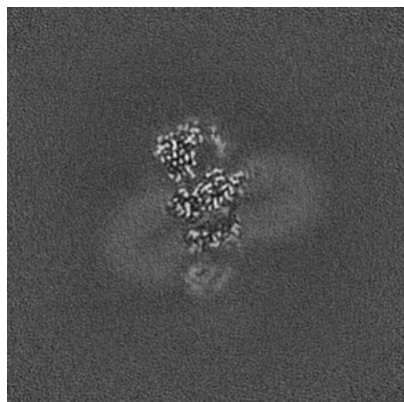


Y Index: 126

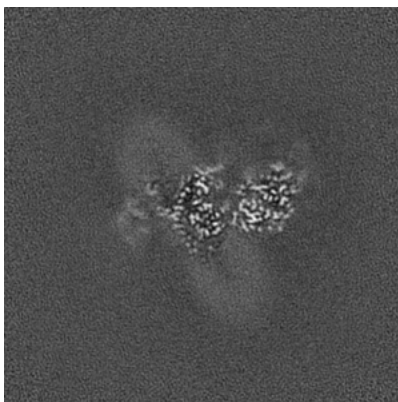


Z Index: 144

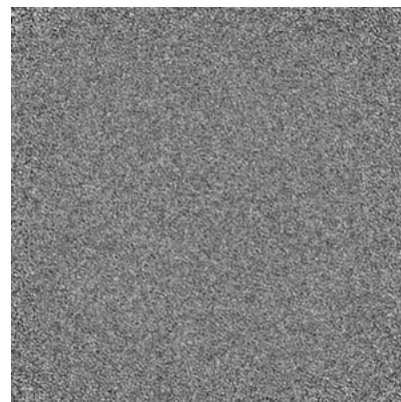
### 6.3.2 Raw map



X Index: 135



Y Index: 130



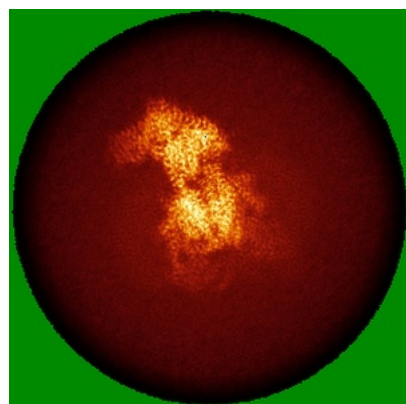
Z Index: 0

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

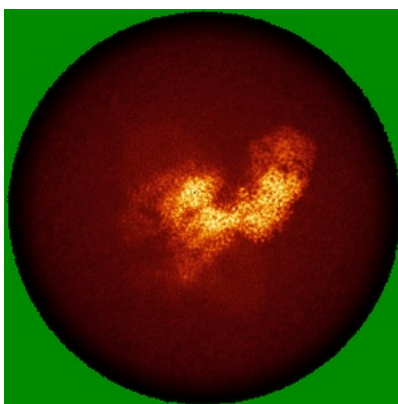


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

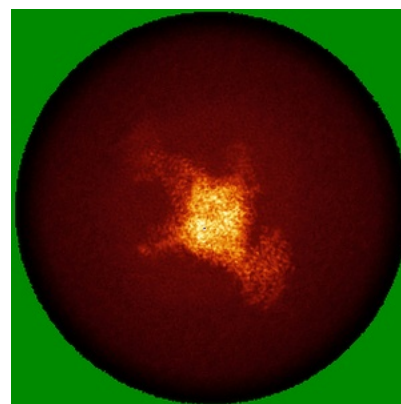
### 6.4.1 Primary map



X

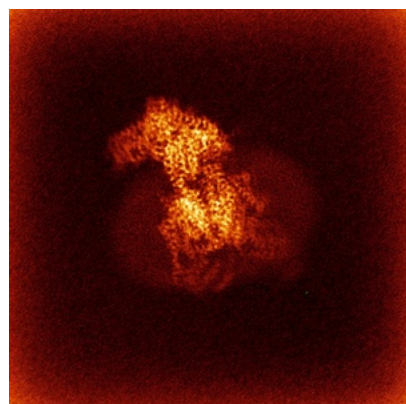


Y

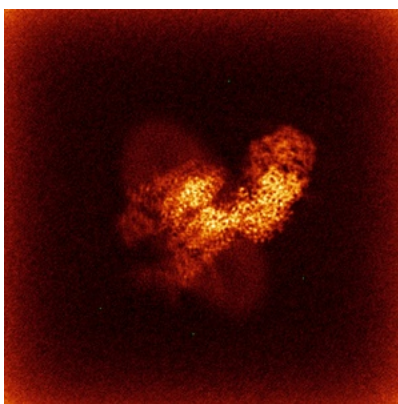


Z

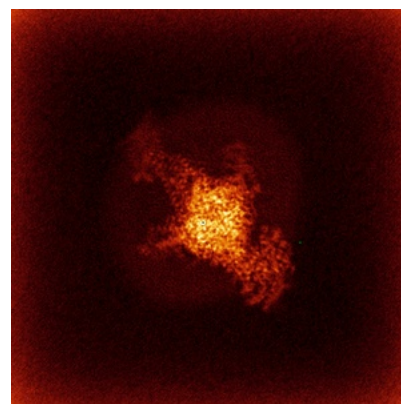
### 6.4.2 Raw map



X



Y

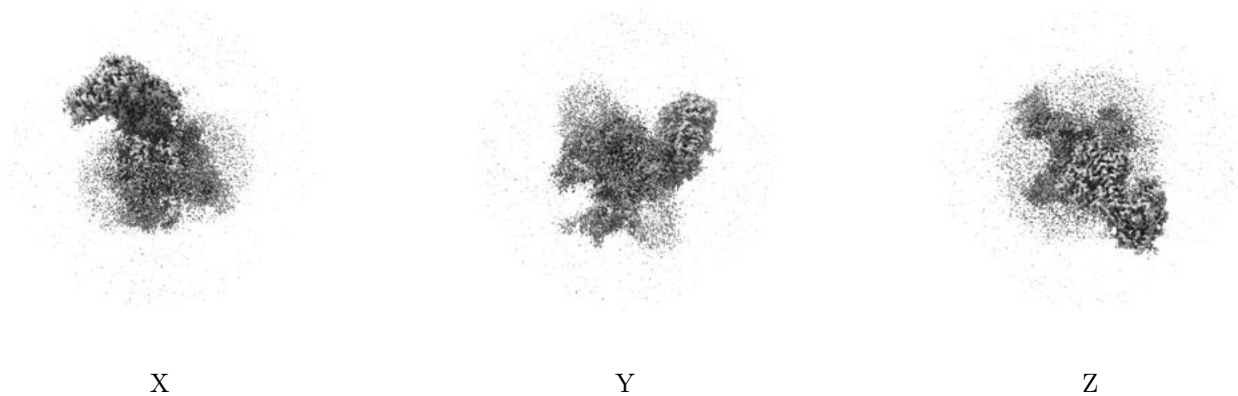


Z

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.

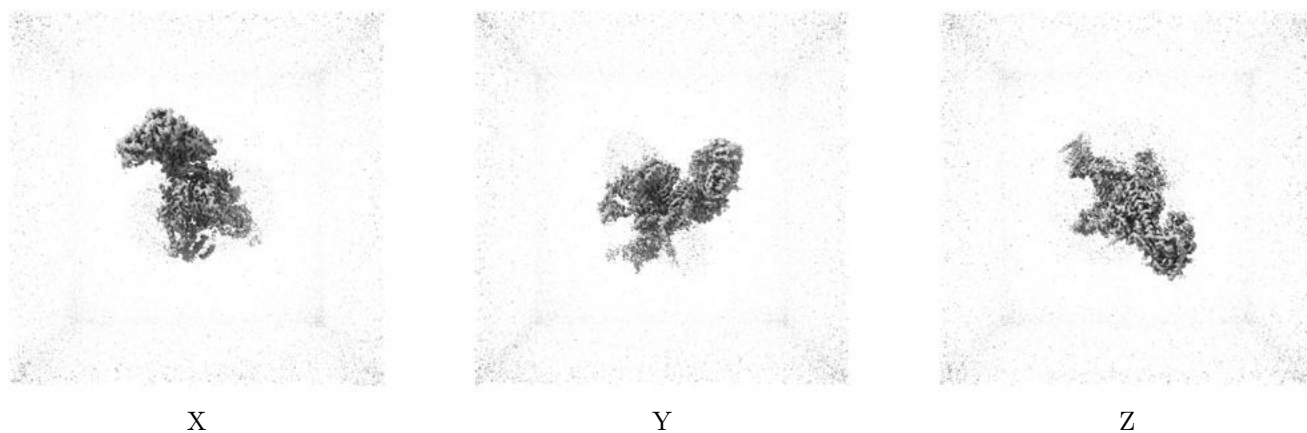
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

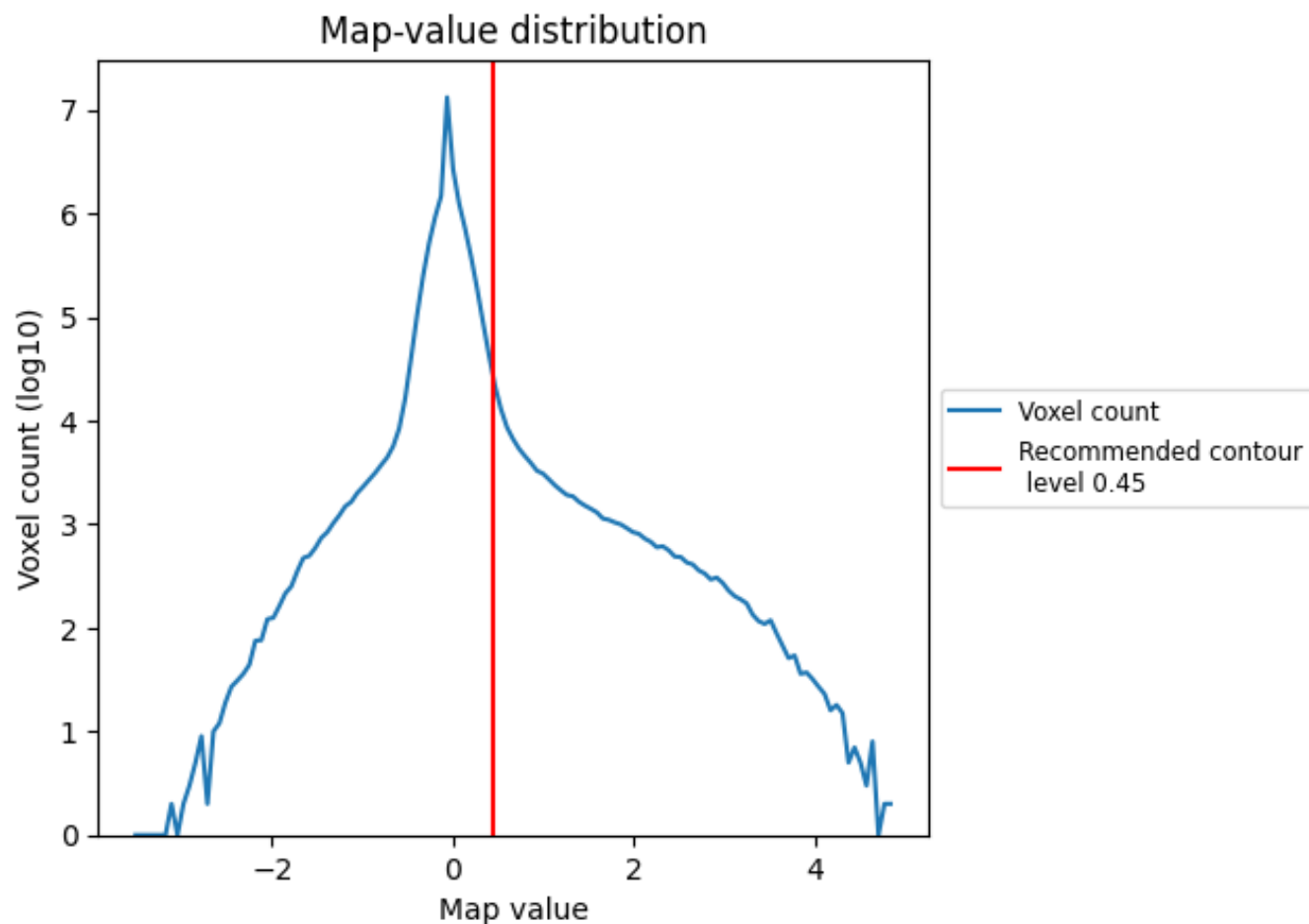
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

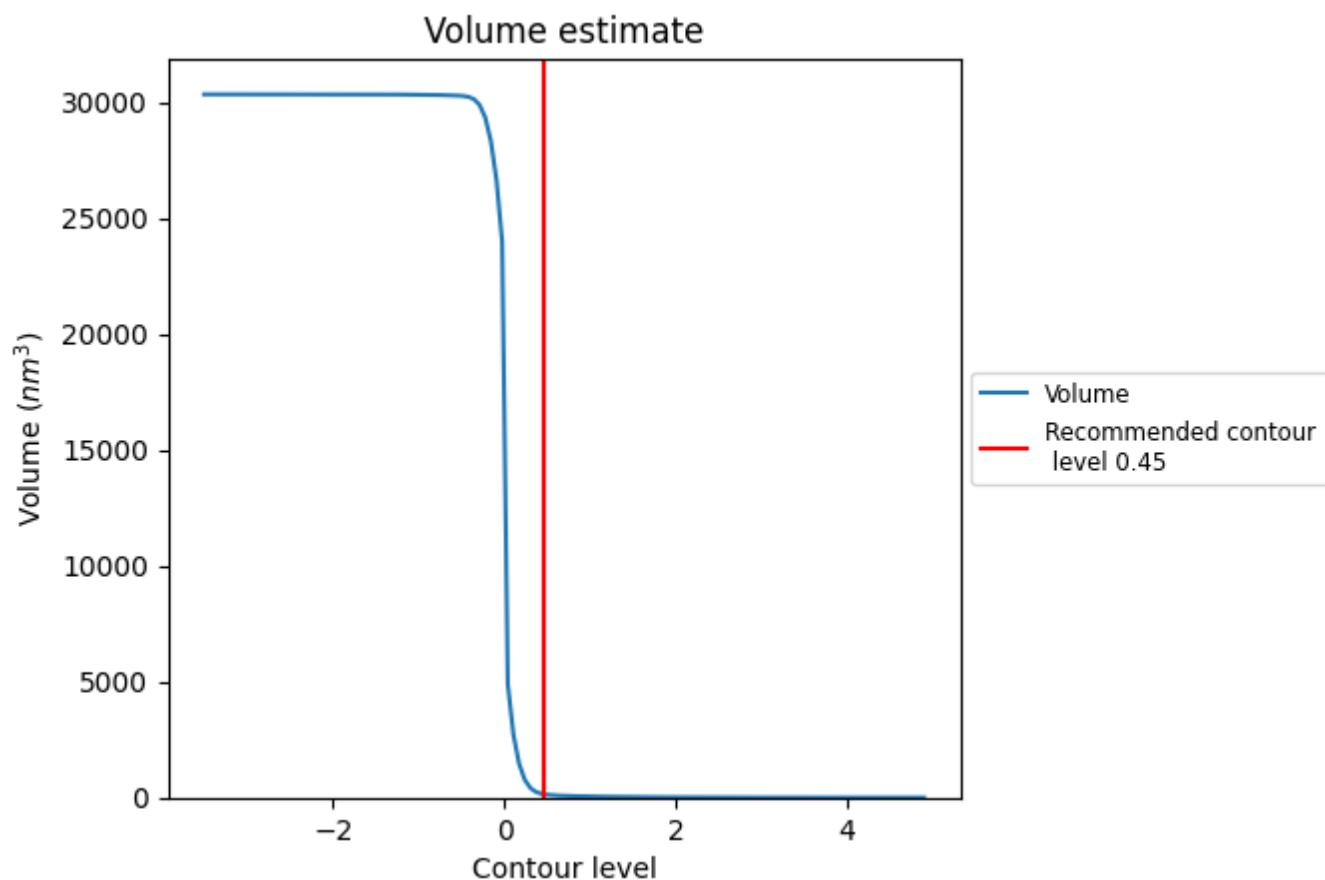
This section contains the results of statistical analysis of the map.

### 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](#)

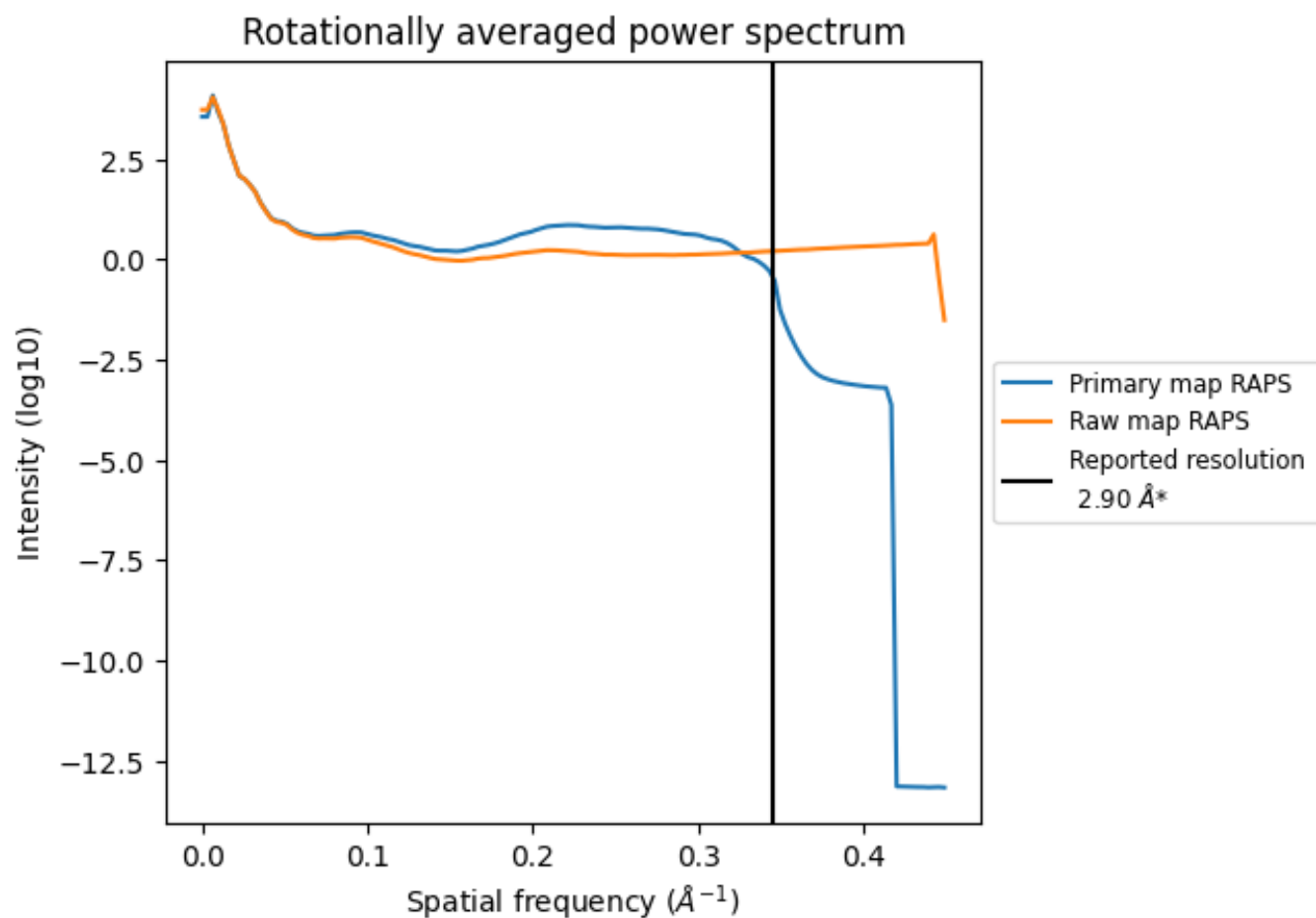


The volume at the recommended contour level is 153 nm<sup>3</sup>; this corresponds to an approximate mass of 138 kDa.

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 ⓘ

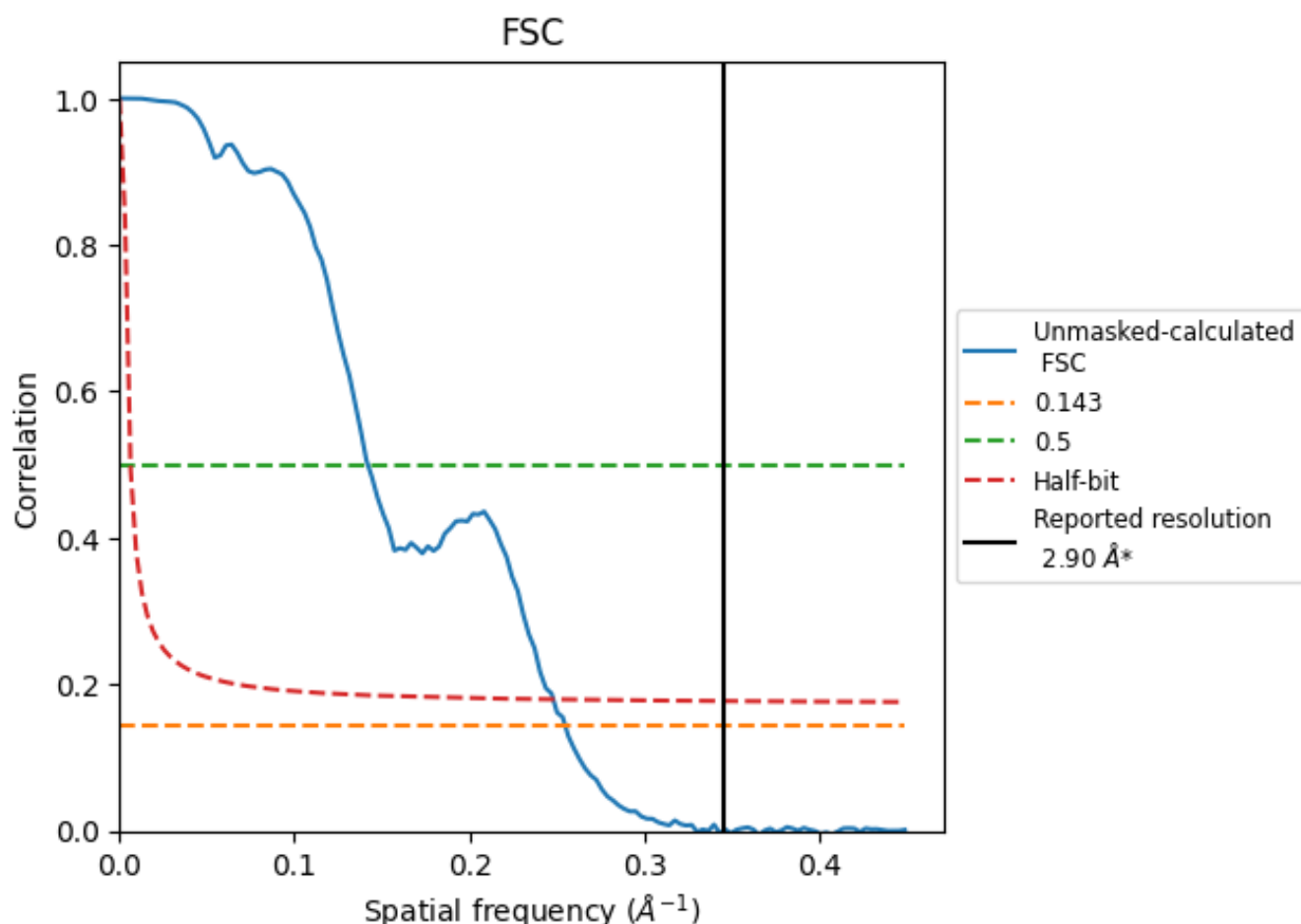


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

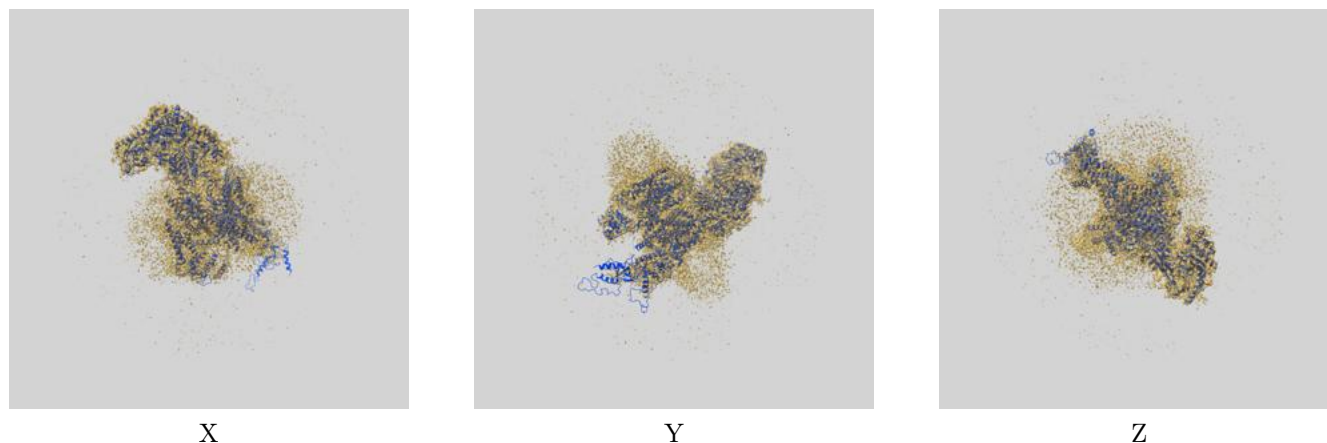
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.05	4.03

\*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 3.92 differs from the reported value 2.9 by more than 10 %

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

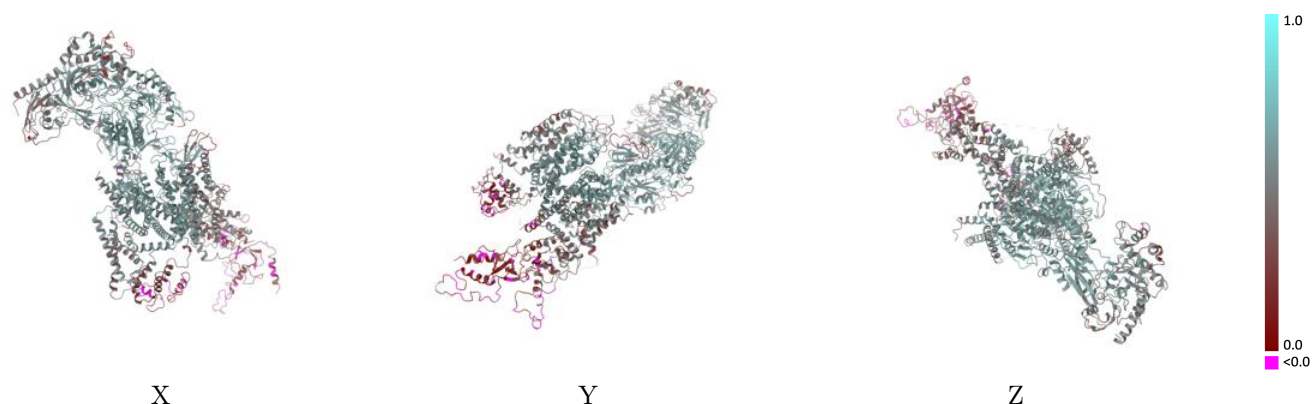
This section contains information regarding the fit between EMDB map EMD-37474 and PDB model 8WE8. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



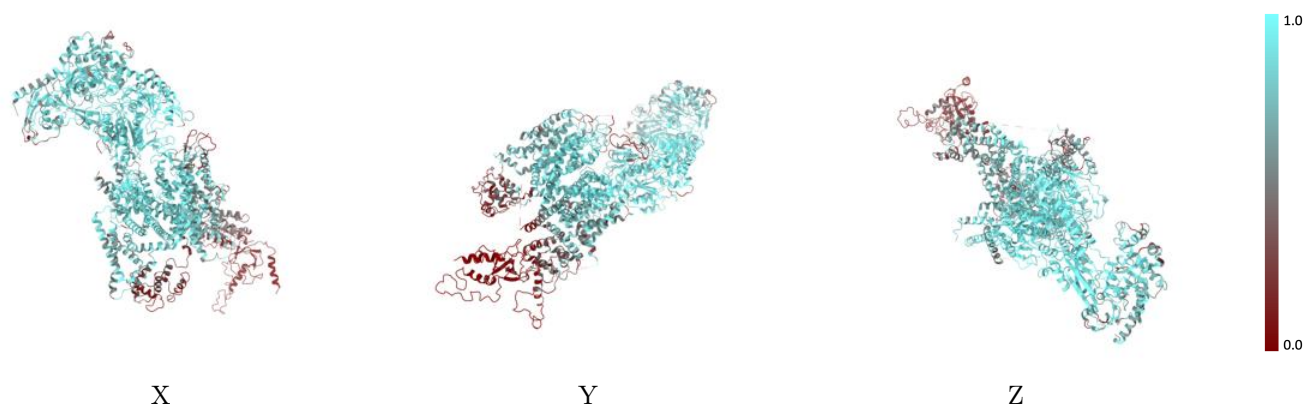
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



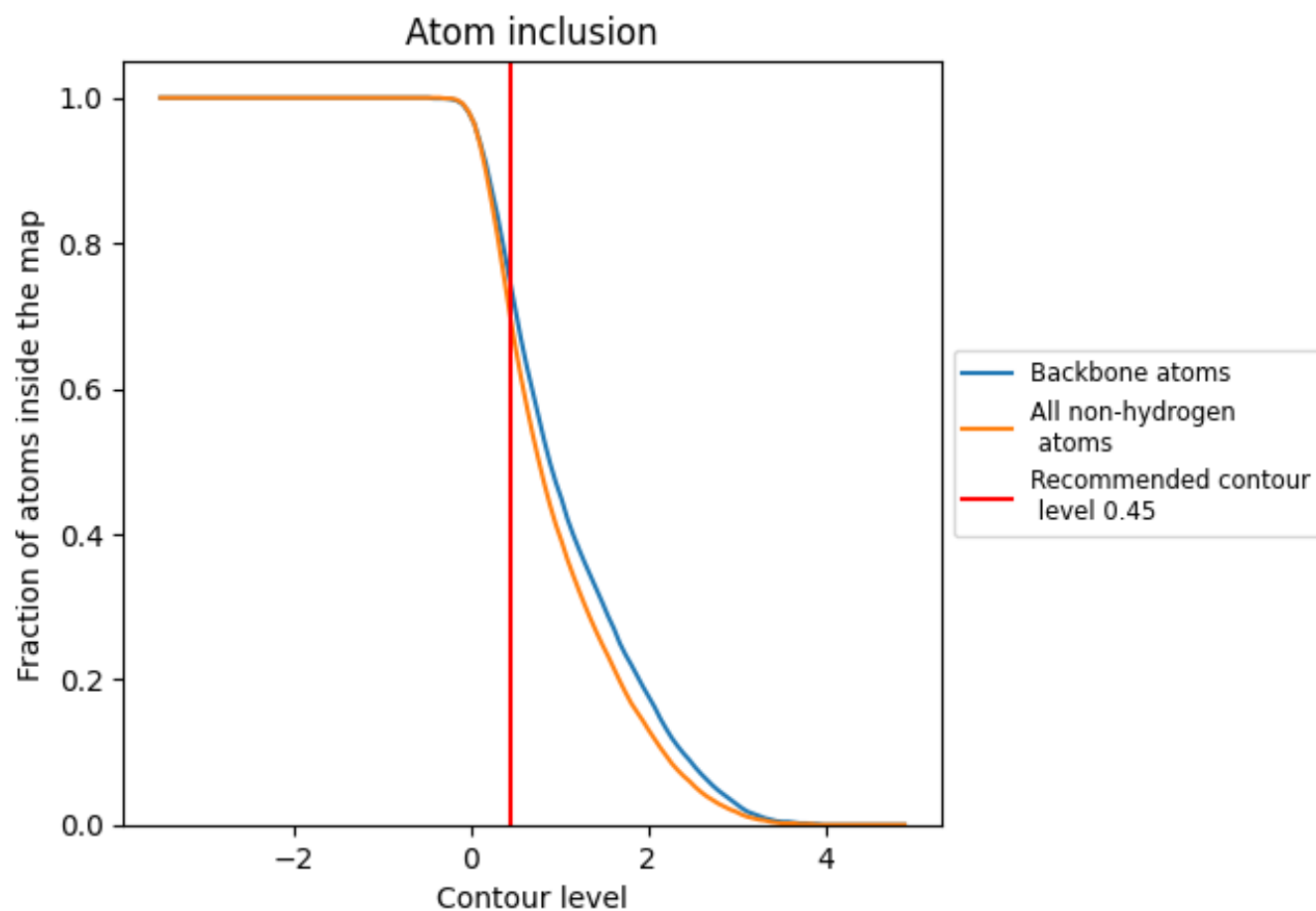
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6950	<div></div> 0.4750
A	<div></div> 0.7370	<div></div> 0.4960
B	<div></div> 0.4100	<div></div> 0.4150
C	<div></div> 0.1690	<div></div> 0.2260
D	<div></div> 0.8380	<div></div> 0.5380
E	<div></div> 0.4760	<div></div> 0.3400
F	<div></div> 0.2500	<div></div> 0.2500
G	<div></div> 0.7500	<div></div> 0.4600
H	<div></div> 0.4290	<div></div> 0.3770
I	<div></div> 0.6070	<div></div> 0.3640

1.0

0.0

<0.0