



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 05:09 AM JST

PDB ID : 8WE6
EMDB ID : EMD-37472
Title : Human L-type voltage-gated calcium channel Cav1.2 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

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 : 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

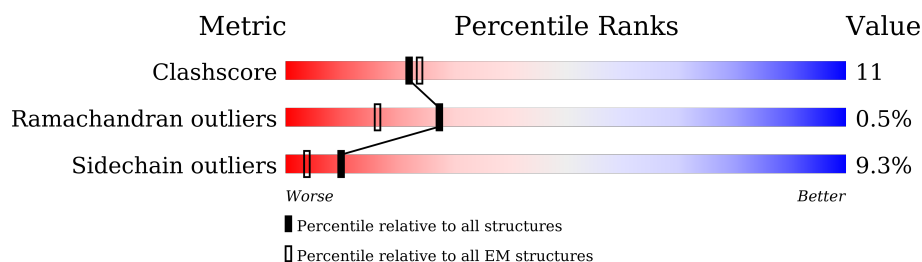
1 Overall quality at a glance

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 ≥ 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	
2	D	1103	
3	C	484	
4	B	3	
5	E	2	
5	G	2	
5	H	2	
6	F	4	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20758 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	1260	Total	C	N	O	S	0	0
			10172	6686	1659	1764	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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



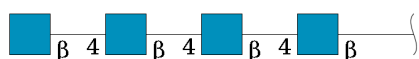
Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			42	24	3	15		

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



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

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

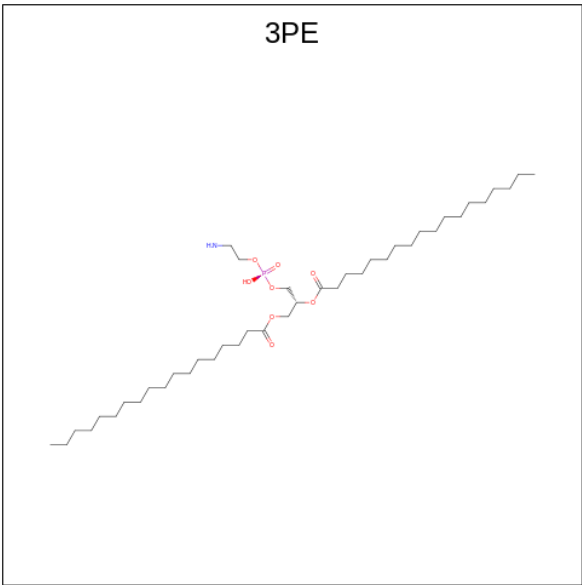


Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

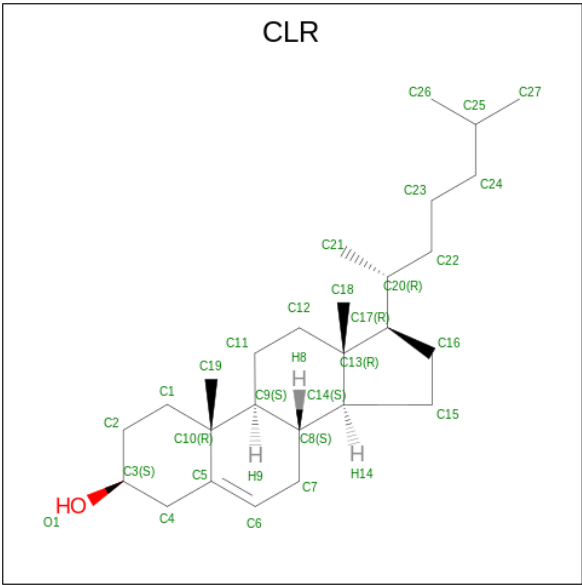
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	D	1	Total	Ca	0
			1	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



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

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



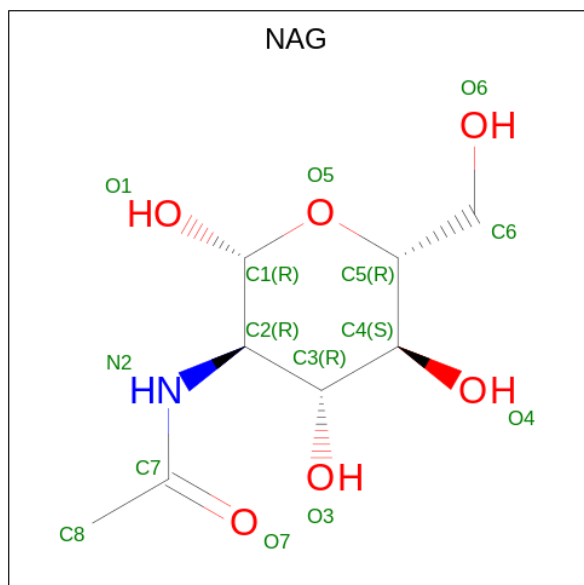
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	

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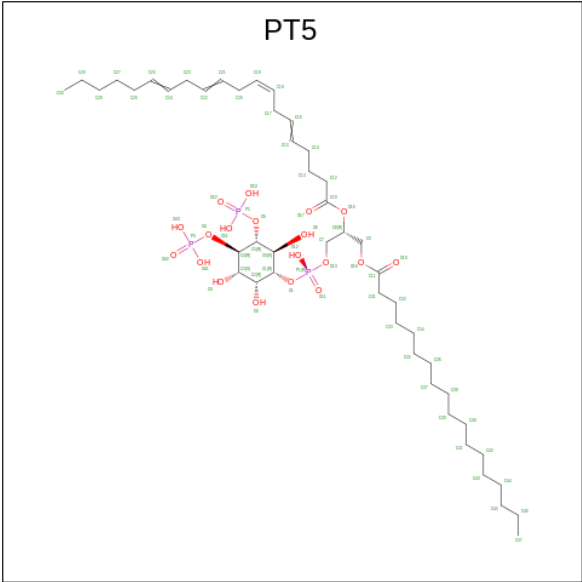
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	

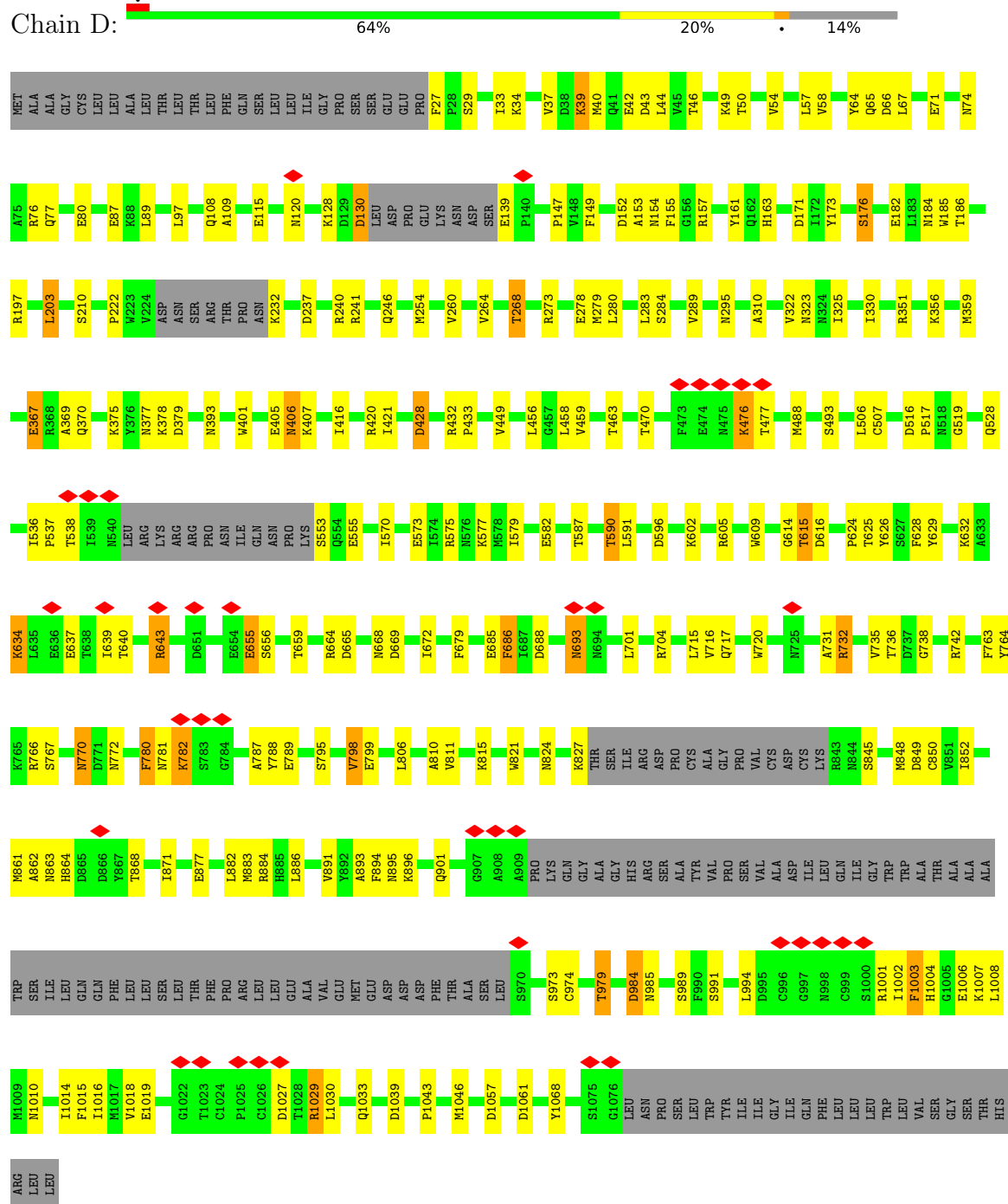
- Molecule 11 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



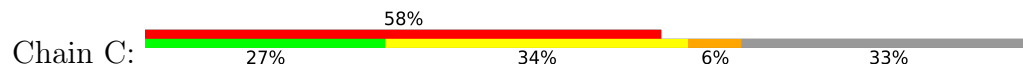
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	A	1	63	41	19	3	0

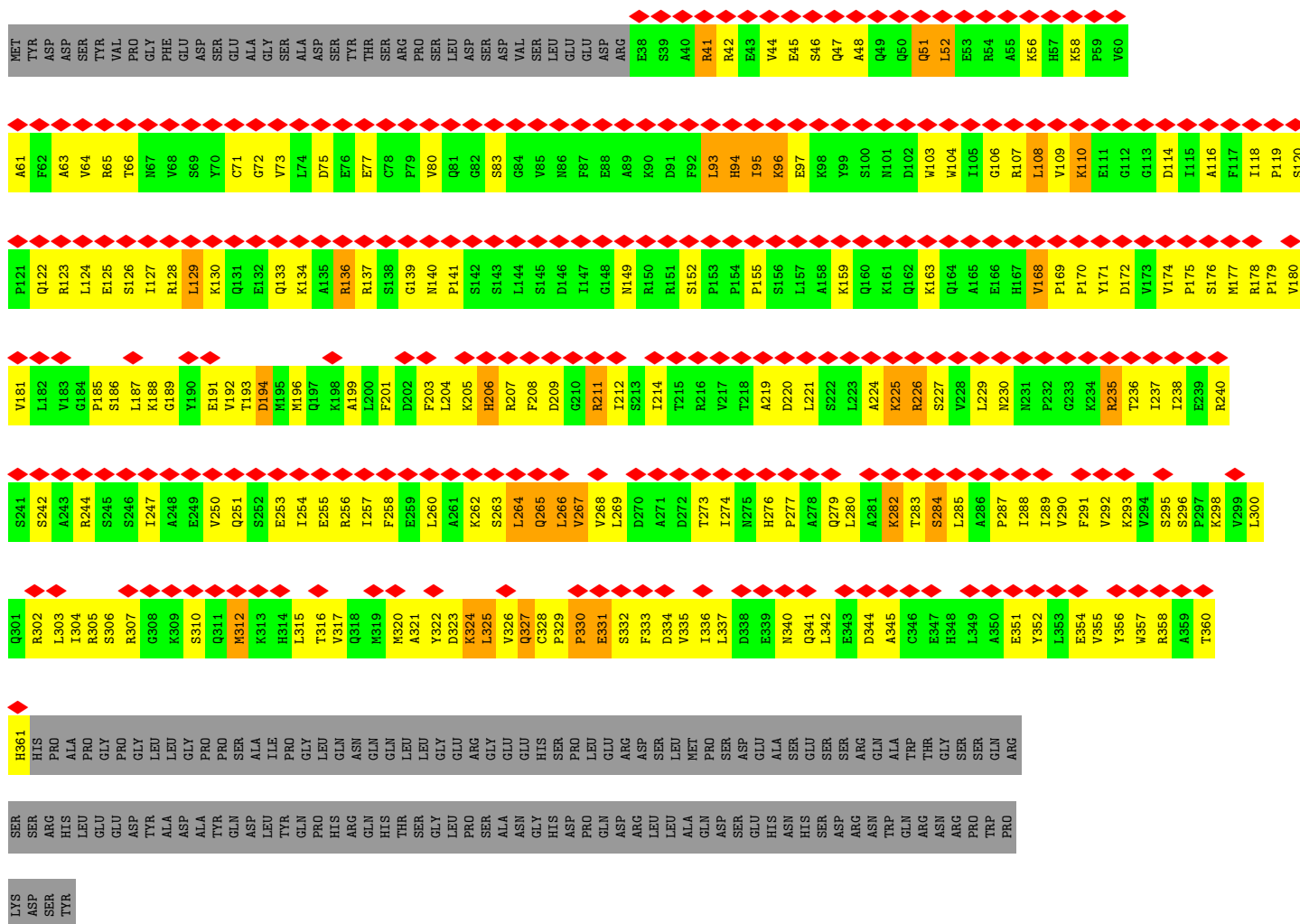


- Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1



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





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



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



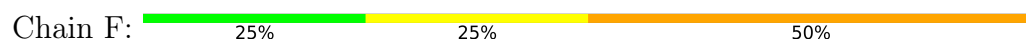
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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-(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	74130	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	4.169	Depositor
Minimum map value	-3.134	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.122	Depositor
Recommended contour level	0.4	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: NAG, CLR, CA, PT5, 3PE

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	0.30	0/10402	0.51	0/14093
2	D	0.26	0/7728	0.49	0/10477
3	C	0.28	0/2624	0.61	0/3544
All	All	0.28	0/20754	0.51	0/28114

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	10172	0	10395	183	0
2	D	7570	0	7369	137	0
3	C	2575	0	2619	148	0
4	B	42	0	37	3	0
5	E	28	0	25	0	0
5	G	28	0	25	1	0
5	H	28	0	25	1	0
6	F	56	0	49	4	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	40	0	54	1	0
9	A	112	0	184	8	0
10	A	14	0	13	0	0
10	D	28	0	26	0	0
11	A	63	0	67	1	0
All	All	20758	0	20888	469	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 11.

All (469) 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)
3:C:330:PRO:HB2	3:C:334:ASP:HA	1.55	0.88
3:C:289:ILE:HD12	3:C:332:SER:HB2	1.63	0.79
1:A:773:LYS:O	1:A:777:LYS:HB3	1.84	0.78
3:C:174:VAL:HG22	3:C:175:PRO:HD2	1.66	0.77
1:A:300:ASN:HB2	1:A:308:PRO:HG2	1.68	0.76
1:A:1569:LEU:HD11	1:A:1613:LEU:HD11	1.66	0.76
1:A:1573:GLN:HB2	1:A:1575:PRO:HD2	1.68	0.75
3:C:180:VAL:HG22	3:C:266:LEU:HB2	1.69	0.75
1:A:1294:LYS:HD3	1:A:1295:PRO:HD2	1.69	0.74
1:A:1570:ARG:H	1:A:1570:ARG:HD2	1.54	0.72
3:C:180:VAL:CG2	3:C:266:LEU:HB2	2.19	0.72
3:C:255:GLU:OE1	3:C:255:GLU:N	2.22	0.70
1:A:621:CYS:C	1:A:623:ARG:H	1.95	0.69
1:A:607:GLU:HG2	1:A:608:THR:HG23	1.73	0.69
1:A:610:ILE:HD12	1:A:610:ILE:H	1.57	0.69
1:A:605:LEU:HB3	1:A:611:MET:HB3	1.75	0.69
1:A:1440:GLU:HG3	1:A:1468:ASP:HB3	1.75	0.68
1:A:1597:PRO:HD2	1:A:1608:ALA:HB1	1.75	0.68
1:A:537:ASN:ND2	1:A:620:ARG:HD2	2.08	0.68
3:C:317:VAL:O	3:C:321:ALA:N	2.25	0.68
2:D:109:ALA:HA	2:D:470:THR:HG22	1.76	0.68
1:A:124:LYS:HB2	1:A:125:PRO:HD3	1.74	0.68
2:D:787:ALA:HB1	2:D:871:ILE:HD11	1.75	0.67
3:C:63:ALA:HB3	3:C:174:VAL:H	1.60	0.67
2:D:184:ASN:HD21	4:B:1:NAG:H62	1.60	0.67
3:C:219:ALA:HB1	3:C:250:VAL:HG23	1.75	0.67
1:A:386:VAL:HG11	8:A:2302:3PE:H371	1.78	0.66
1:A:430:LEU:HD11	3:C:298:LYS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:528:GLN:O	2:D:901:GLN:NE2	2.29	0.66
1:A:777:LYS:NZ	3:C:351:GLU:OE2	2.28	0.66
3:C:253:GLU:HA	3:C:256:ARG:HG3	1.76	0.66
1:A:444:ALA:HB2	3:C:199:ALA:HB2	1.76	0.65
2:D:640:THR:HA	2:D:643:ARG:HE	1.61	0.65
3:C:257:ILE:HG22	3:C:258:PHE:H	1.60	0.65
1:A:266:VAL:HG23	1:A:267:PRO:HD3	1.77	0.65
1:A:1217:ARG:O	1:A:1546:LYS:NZ	2.25	0.65
3:C:323:ASP:HA	3:C:326:VAL:HG12	1.78	0.65
3:C:221:LEU:HD12	3:C:280:LEU:HD13	1.78	0.65
3:C:209:ASP:H	3:C:212:ILE:HB	1.59	0.65
1:A:1479:CYS:N	1:A:1495:CYS:SG	2.70	0.64
3:C:291:PHE:HE2	3:C:325:LEU:HB3	1.62	0.64
1:A:1598:LEU:HD21	1:A:1649:LEU:HD12	1.80	0.64
3:C:181:VAL:HG11	3:C:274:ILE:HD13	1.79	0.64
3:C:300:LEU:HA	3:C:303:LEU:HB2	1.79	0.64
2:D:351:ARG:HH22	2:D:356:LYS:HD3	1.62	0.64
2:D:65:GLN:OE1	2:D:65:GLN:N	2.21	0.63
1:A:147:PHE:HB3	1:A:151:ASP:HB3	1.79	0.63
3:C:293:LYS:HD2	3:C:336:ILE:HD11	1.81	0.63
1:A:1083:LYS:HD2	1:A:1088:GLU:HG2	1.80	0.63
2:D:655:GLU:O	2:D:717:GLN:NE2	2.32	0.63
2:D:716:VAL:HA	2:D:720:TRP:HB2	1.81	0.63
1:A:1280:GLY:O	1:A:1284:VAL:HG13	1.99	0.62
3:C:226:ARG:NH1	3:C:283:THR:OG1	2.32	0.62
1:A:1122:LEU:HG	9:A:2303:CLR:H151	1.81	0.62
2:D:115:GLU:OE2	6:F:3:NAG:O3	2.17	0.62
1:A:1590:ARG:HA	1:A:1593:SER:HB2	1.82	0.62
2:D:637:GLU:HG2	2:D:640:THR:HG23	1.81	0.62
1:A:764:SER:O	1:A:768:GLU:HG2	1.99	0.62
1:A:635:ASN:O	1:A:639:ASN:ND2	2.32	0.61
1:A:537:ASN:ND2	1:A:620:ARG:HH11	1.97	0.61
1:A:1418:LEU:HD22	1:A:1514:LEU:HD12	1.82	0.61
3:C:247:ILE:HA	3:C:250:VAL:HG12	1.81	0.61
1:A:366:THR:HG21	1:A:1459:ARG:HG3	1.82	0.61
1:A:1201:GLU:CD	1:A:1202:LEU:H	2.02	0.61
2:D:979:THR:O	2:D:1033:GLN:NE2	2.23	0.61
1:A:1557:LYS:HG2	1:A:1559:ARG:HG2	1.81	0.61
1:A:1190:GLN:O	1:A:1194:GLU:HB3	2.01	0.60
1:A:1053:VAL:O	1:A:1057:THR:OG1	2.20	0.60
3:C:251:GLN:HA	3:C:254:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:VAL:HG11	2:D:1006:GLU:HG2	1.82	0.60
3:C:63:ALA:HA	3:C:94:HIS:HA	1.83	0.60
1:A:537:ASN:HD22	1:A:620:ARG:HD2	1.67	0.60
1:A:679:PHE:HD2	1:A:685:ARG:HE	1.49	0.60
3:C:119:PRO:HB3	3:C:123:ARG:HG2	1.84	0.60
3:C:185:PRO:HD2	3:C:193:THR:HA	1.84	0.60
1:A:537:ASN:HD21	1:A:620:ARG:HH11	1.49	0.59
1:A:1221:ARG:HD3	1:A:1550:ALA:HB1	1.84	0.59
1:A:1422:TYR:HH	1:A:1506:SER:HG	1.49	0.59
1:A:1064:ALA:O	1:A:1068:VAL:HG23	2.03	0.59
1:A:536:LEU:O	1:A:540:THR:HG23	2.03	0.59
1:A:1074:LYS:HB3	1:A:1147:SER:HB2	1.84	0.59
3:C:302:ARG:HA	3:C:305:ARG:HG2	1.84	0.59
1:A:621:CYS:O	1:A:623:ARG:N	2.36	0.59
3:C:300:LEU:O	3:C:304:ILE:HG13	2.01	0.59
2:D:994:LEU:N	2:D:1001:ARG:O	2.30	0.59
3:C:358:ARG:O	3:C:361:HIS:ND1	2.33	0.59
3:C:332:SER:C	3:C:334:ASP:H	2.06	0.58
2:D:153:ALA:O	2:D:155:PHE:N	2.37	0.58
2:D:536:ILE:HD12	2:D:536:ILE:H	1.67	0.58
1:A:1245:MET:O	1:A:1249:ILE:HG13	2.03	0.58
3:C:64:VAL:HG13	3:C:171:TYR:HB3	1.86	0.58
1:A:756:LEU:O	1:A:760:GLU:HG2	2.04	0.58
3:C:186:SER:OG	3:C:187:LEU:N	2.37	0.57
3:C:207:ARG:O	3:C:207:ARG:NH1	2.33	0.57
1:A:1277:LEU:O	1:A:1281:LEU:HG	2.05	0.57
2:D:39:LYS:NZ	2:D:824:ASN:O	2.38	0.57
3:C:178:ARG:NH1	3:C:356:TYR:OH	2.38	0.57
2:D:155:PHE:HA	2:D:456:LEU:HD11	1.86	0.56
2:D:1027:ASP:OD1	2:D:1027:ASP:N	2.38	0.56
2:D:37:VAL:HG21	2:D:1006:GLU:HB3	1.86	0.56
2:D:240:ARG:NH2	2:D:278:GLU:O	2.38	0.56
3:C:71:CYS:SG	3:C:72:GLY:N	2.77	0.56
1:A:1030:ASN:OD1	1:A:1036:LYS:NZ	2.38	0.56
1:A:1596:MET:SD	1:A:1596:MET:N	2.79	0.56
3:C:188:LYS:NZ	3:C:274:ILE:O	2.38	0.56
1:A:237:ARG:HH11	1:A:240:ARG:HH12	1.52	0.56
1:A:431:GLU:HA	1:A:434:LEU:HB2	1.88	0.56
1:A:923:VAL:HB	1:A:1482:GLU:HG3	1.88	0.55
1:A:1269:ILE:O	1:A:1273:ILE:HG12	2.06	0.55
3:C:283:THR:OG1	3:C:284:SER:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:163:GLU:HG2	2.05	0.55
3:C:93:LEU:HB3	3:C:108:LEU:HD22	1.87	0.55
3:C:58:LYS:HZ3	3:C:107:ARG:HE	1.55	0.55
2:D:537:PRO:HD3	2:D:974:CYS:HB3	1.89	0.55
3:C:256:ARG:HA	3:C:260:LEU:HD13	1.89	0.55
2:D:659:THR:OG1	2:D:742:ARG:NH1	2.40	0.55
6:F:4:NAG:H3	6:F:4:NAG:H83	1.88	0.55
1:A:1480:ALA:O	1:A:1481:PRO:C	2.45	0.54
2:D:615:THR:OG1	2:D:616:ASP:N	2.40	0.54
3:C:221:LEU:HA	3:C:224:ALA:HB3	1.88	0.54
3:C:328:CYS:HB2	3:C:329:PRO:HD2	1.90	0.54
2:D:693:ASN:C	2:D:693:ASN:HD22	2.10	0.54
3:C:289:ILE:O	3:C:333:PHE:HA	2.06	0.54
1:A:961:THR:O	1:A:965:THR:OG1	2.23	0.54
3:C:330:PRO:O	3:C:332:SER:N	2.33	0.54
1:A:952:ILE:HD12	1:A:952:ILE:H	1.71	0.53
1:A:1560:ILE:HG13	1:A:1604:VAL:HG12	1.90	0.53
1:A:621:CYS:C	1:A:623:ARG:N	2.62	0.53
2:D:428:ASP:OD1	2:D:428:ASP:N	2.41	0.53
3:C:312:MET:SD	3:C:312:MET:N	2.76	0.53
1:A:427:LYS:NZ	1:A:431:GLU:OE1	2.36	0.53
1:A:729:VAL:HB	9:A:2304:CLR:H151	1.90	0.53
3:C:326:VAL:O	3:C:327:GLN:C	2.47	0.53
2:D:1061:ASP:OD1	2:D:1061:ASP:N	2.41	0.53
3:C:321:ALA:O	3:C:325:LEU:HD12	2.09	0.53
3:C:108:LEU:HD12	3:C:110:LYS:HD2	1.90	0.53
2:D:770:ASN:N	2:D:770:ASN:OD1	2.41	0.53
1:A:1548:ILE:HD11	1:A:1571:ARG:HB3	1.90	0.53
3:C:127:ILE:HG23	3:C:130:LYS:HD3	1.91	0.53
3:C:136:ARG:HG3	3:C:137:ARG:H	1.74	0.53
2:D:39:LYS:HD2	2:D:40:MET:HG3	1.91	0.52
3:C:75:ASP:OD1	3:C:123:ARG:NH2	2.42	0.52
1:A:1212:TYR:CD1	1:A:1542:LEU:HD21	2.44	0.52
3:C:44:VAL:O	3:C:47:GLN:N	2.39	0.52
3:C:56:LYS:O	3:C:107:ARG:NH2	2.43	0.52
3:C:139:GLY:HA3	3:C:155:PRO:HD2	1.90	0.52
3:C:220:ASP:HA	3:C:273:THR:HG22	1.92	0.52
3:C:317:VAL:HA	3:C:320:MET:HB3	1.92	0.52
1:A:151:ASP:OD1	1:A:152:SER:N	2.42	0.52
1:A:1137:TRP:CD1	1:A:1138:PRO:HD3	2.45	0.52
3:C:180:VAL:HG21	3:C:266:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:290:VAL:HA	3:C:335:VAL:HB	1.92	0.52
3:C:291:PHE:CE2	3:C:325:LEU:HB3	2.44	0.52
6:F:3:NAG:H83	6:F:3:NAG:H3	1.90	0.52
3:C:137:ARG:HB3	3:C:141:PRO:O	2.10	0.52
1:A:1489:THR:C	1:A:1491:GLY:H	2.13	0.51
3:C:61:ALA:HB3	3:C:96:LYS:HB3	1.91	0.51
3:C:316:THR:O	3:C:320:MET:N	2.44	0.51
1:A:1466:TRP:HA	1:A:1469:ILE:HD12	1.92	0.51
3:C:123:ARG:HD2	3:C:127:ILE:HG12	1.92	0.51
1:A:251:VAL:HG22	1:A:253:SER:H	1.75	0.51
1:A:510:ASN:HB3	1:A:514:ARG:HG3	1.92	0.51
1:A:998:SER:O	1:A:1002:ILE:HG23	2.10	0.51
3:C:277:PRO:HG3	3:C:333:PHE:CD2	2.45	0.51
1:A:1013:VAL:O	1:A:1017:LEU:N	2.44	0.51
1:A:1492:GLU:HG2	1:A:1493:THR:H	1.75	0.51
1:A:1570:ARG:HH22	1:A:1588:CYS:HB2	1.75	0.51
1:A:1434:ALA:HB2	1:A:1479:CYS:O	2.11	0.51
1:A:1570:ARG:HH12	1:A:1583:PRO:HA	1.76	0.51
3:C:94:HIS:HD2	3:C:176:SER:HA	1.76	0.51
2:D:637:GLU:HG3	2:D:639:ILE:H	1.77	0.50
1:A:1060:GLN:HG2	1:A:1125:MET:HE3	1.93	0.50
2:D:58:VAL:HG12	2:D:798:VAL:HB	1.93	0.50
3:C:189:GLY:N	3:C:194:ASP:OD2	2.45	0.50
1:A:1052:ILE:O	1:A:1056:THR:OG1	2.20	0.50
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.93	0.50
1:A:299:TYR:HA	1:A:308:PRO:HD2	1.93	0.50
1:A:729:VAL:HB	9:A:2304:CLR:H72	1.93	0.50
1:A:999:VAL:O	1:A:1003:SER:OG	2.28	0.50
3:C:41:ARG:O	3:C:45:GLU:HB2	2.12	0.50
2:D:379:ASP:OD1	2:D:379:ASP:N	2.35	0.50
3:C:185:PRO:HG3	3:C:196:MET:HG3	1.92	0.50
1:A:199:ASP:OD2	1:A:246:ARG:NH1	2.45	0.50
1:A:604:ILE:HA	1:A:607:GLU:HB3	1.94	0.50
2:D:120:ASN:HD21	4:B:1:NAG:H61	1.76	0.50
2:D:862:ALA:H	2:D:868:THR:HG22	1.77	0.50
1:A:537:ASN:HD21	1:A:620:ARG:NH1	2.09	0.50
1:A:1121:VAL:O	1:A:1125:MET:HG3	2.11	0.49
2:D:893:ALA:HB2	2:D:984:ASP:OD1	2.12	0.49
2:D:895:ASN:OD1	5:H:1:NAG:H2	2.11	0.49
3:C:177:MET:HG2	3:C:265:GLN:C	2.32	0.49
1:A:620:ARG:O	1:A:623:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:421:ILE:H	2:D:421:ILE:HD12	1.77	0.49
1:A:1590:ARG:O	1:A:1594:MET:HG2	2.11	0.49
2:D:87:GLU:HG3	2:D:614:GLY:H	1.77	0.49
2:D:688:ASP:OD1	2:D:688:ASP:N	2.36	0.49
1:A:686:ARG:NH2	1:A:1146:ASP:OD1	2.45	0.49
2:D:57:LEU:HD22	2:D:715:LEU:HD22	1.95	0.49
3:C:240:ARG:HG3	3:C:242:SER:H	1.78	0.49
3:C:289:ILE:HB	3:C:333:PHE:HA	1.94	0.49
2:D:171:ASP:OD2	2:D:420:ARG:NH2	2.46	0.49
2:D:896:LYS:HG2	2:D:979:THR:HG23	1.94	0.49
3:C:97:GLU:O	3:C:104:TRP:NE1	2.46	0.49
3:C:104:TRP:HB3	3:C:118:ILE:HD12	1.95	0.49
1:A:1224:PRO:HG2	1:A:1233:TRP:CG	2.47	0.49
3:C:293:LYS:HG3	3:C:295:SER:H	1.78	0.49
2:D:37:VAL:HG13	2:D:1008:LEU:HD13	1.95	0.49
2:D:393:ASN:OD1	2:D:393:ASN:N	2.43	0.49
3:C:66:THR:HA	3:C:171:TYR:CD1	2.48	0.49
2:D:74:ASN:HB3	2:D:77:GLN:HB2	1.95	0.48
2:D:789:GLU:OE1	2:D:789:GLU:N	2.45	0.48
3:C:108:LEU:HB2	3:C:116:ALA:HB2	1.95	0.48
1:A:1206:GLN:HE21	1:A:1210:VAL:HG21	1.79	0.48
2:D:1057:ASP:OD1	2:D:1057:ASP:N	2.37	0.48
3:C:212:ILE:HG13	3:C:214:ILE:HG23	1.95	0.48
2:D:147:PRO:HG2	2:D:149:PHE:CZ	2.48	0.48
1:A:152:SER:OG	1:A:153:ASN:N	2.47	0.48
1:A:277:PHE:CD1	1:A:1388:LEU:HB2	2.48	0.48
3:C:221:LEU:HD11	3:C:285:LEU:HG	1.95	0.48
1:A:1549:TRP:CZ2	1:A:1560:ILE:HD12	2.49	0.48
3:C:125:GLU:HG2	3:C:170:PRO:HG3	1.96	0.48
3:C:178:ARG:CZ	3:C:288:ILE:HG12	2.44	0.48
3:C:324:LYS:HB3	3:C:324:LYS:HE3	1.62	0.48
1:A:899:ASP:HB3	1:A:902:PHE:HB3	1.96	0.48
3:C:344:ASP:OD2	3:C:344:ASP:N	2.40	0.48
1:A:637:LEU:HD11	1:A:1051:ASN:HB3	1.96	0.48
1:A:1225:LYS:HG2	1:A:1226:ASN:H	1.78	0.48
1:A:380:TRP:N	1:A:381:PRO:HD3	2.29	0.47
1:A:952:ILE:O	1:A:956:ALA:N	2.35	0.47
2:D:27:PHE:HZ	2:D:1004:HIS:HB2	1.79	0.47
2:D:152:ASP:OD2	2:D:153:ALA:N	2.47	0.47
3:C:237:ILE:HA	3:C:244:ARG:HH12	1.79	0.47
1:A:614:LEU:HD13	1:A:1070:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:GLU:HG3	2:D:632:LYS:HE3	1.97	0.47
3:C:48:ALA:O	3:C:52:LEU:HD12	2.15	0.47
3:C:277:PRO:HG3	3:C:333:PHE:HD2	1.79	0.47
2:D:517:PRO:HA	2:D:579:ILE:HG23	1.95	0.47
2:D:664:ARG:NH1	2:D:738:GLY:O	2.48	0.47
1:A:554:GLU:HA	1:A:557:ASP:OD1	2.13	0.47
1:A:1390:ARG:HD2	1:A:1391:GLY:H	1.80	0.47
2:D:280:LEU:HA	2:D:283:LEU:HD12	1.96	0.47
2:D:605:ARG:HD3	2:D:624:PRO:HB3	1.95	0.47
2:D:985:ASN:OD1	2:D:985:ASN:N	2.45	0.47
3:C:257:ILE:HG22	3:C:258:PHE:N	2.26	0.47
3:C:276:HIS:CD2	3:C:277:PRO:HD2	2.49	0.47
1:A:622:VAL:HG22	1:A:1062:MET:SD	2.55	0.47
1:A:1310:ILE:HG21	1:A:1383:ARG:HG3	1.96	0.47
1:A:1549:TRP:CH2	1:A:1560:ILE:HG23	2.49	0.47
2:D:693:ASN:C	2:D:693:ASN:ND2	2.68	0.47
2:D:260:VAL:HG23	2:D:295:ASN:HB3	1.97	0.47
2:D:570:ILE:O	2:D:573:GLU:HG3	2.15	0.47
3:C:129:LEU:O	3:C:133:GLN:N	2.48	0.47
1:A:131:LEU:HD11	1:A:250:GLY:HA3	1.96	0.47
2:D:863:ASN:OD1	2:D:864:HIS:N	2.47	0.47
3:C:229:LEU:HD23	3:C:230:ASN:HB2	1.97	0.47
5:G:1:NAG:H61	5:G:2:NAG:N2	2.29	0.47
1:A:1260:HIS:CG	9:A:2306:CLR:H12	2.49	0.46
2:D:852:ILE:HD11	2:D:861:MET:HG2	1.96	0.46
1:A:1424:VAL:O	1:A:1428:GLN:HG2	2.15	0.46
1:A:1585:ARG:HD3	1:A:1586:VAL:HG12	1.96	0.46
2:D:616:ASP:N	2:D:616:ASP:OD1	2.48	0.46
1:A:992:LEU:O	1:A:996:VAL:HG23	2.16	0.46
2:D:1007:LYS:HG2	2:D:1014:ILE:HG13	1.96	0.46
1:A:1205:ASN:ND2	1:A:1537:LEU:O	2.24	0.46
9:A:2306:CLR:H221	9:A:2306:CLR:H162	1.42	0.46
3:C:211:ARG:HH12	3:C:265:GLN:HA	1.81	0.46
2:D:42:GLU:O	2:D:46:THR:OG1	2.20	0.46
2:D:459:VAL:HG12	2:D:493:SER:HA	1.96	0.46
3:C:341:GLN:CD	3:C:341:GLN:H	2.19	0.46
3:C:124:LEU:HD13	3:C:171:TYR:OH	2.16	0.46
9:A:2305:CLR:H162	9:A:2305:CLR:H221	1.66	0.46
2:D:182:GLU:O	2:D:186:THR:OG1	2.25	0.46
2:D:577:LYS:HE3	2:D:609:TRP:HZ2	1.81	0.46
3:C:352:TYR:O	3:C:356:TYR:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:LYS:O	2:D:43:ASP:HB2	2.15	0.46
2:D:886:LEU:HD22	2:D:891:VAL:HG21	1.96	0.46
1:A:529:LEU:O	1:A:533:LEU:HG	2.16	0.46
2:D:76:ARG:O	2:D:80:GLU:HG2	2.16	0.46
2:D:157:ARG:NH2	2:D:222:PRO:O	2.49	0.46
3:C:333:PHE:O	3:C:334:ASP:C	2.54	0.46
1:A:767:LYS:HE2	1:A:767:LYS:HB3	1.57	0.45
1:A:1489:THR:OG1	1:A:1490:GLU:N	2.48	0.45
2:D:367:GLU:OE2	2:D:369:ALA:N	2.45	0.45
2:D:668:ASN:OD1	2:D:668:ASN:N	2.41	0.45
3:C:71:CYS:SG	3:C:73:VAL:HG23	2.56	0.45
3:C:291:PHE:HB3	3:C:336:ILE:HD12	1.98	0.45
3:C:332:SER:C	3:C:334:ASP:N	2.70	0.45
1:A:968:ILE:HD13	1:A:968:ILE:HA	1.67	0.45
1:A:1218:PRO:HB2	1:A:1556:ALA:HA	1.97	0.45
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.52	0.45
2:D:161:TYR:HB3	2:D:197:ARG:NH2	2.32	0.45
2:D:519:GLY:HA3	2:D:575:ARG:HH21	1.81	0.45
3:C:125:GLU:O	3:C:128:ARG:HG2	2.16	0.45
1:A:1532:ARG:HD3	1:A:1540:HIS:CD2	2.51	0.45
2:D:44:LEU:HD11	2:D:821:TRP:HE1	1.80	0.45
3:C:357:TRP:O	3:C:360:THR:OG1	2.33	0.45
1:A:425:ARG:NH2	1:A:769:GLU:OE1	2.50	0.45
1:A:1570:ARG:HH12	1:A:1583:PRO:CA	2.30	0.45
2:D:799:GLU:HG2	2:D:806:LEU:HD11	1.98	0.45
3:C:124:LEU:HD22	3:C:171:TYR:CE1	2.51	0.45
1:A:1012:ASN:HA	1:A:1015:LYS:NZ	2.31	0.45
1:A:617:SER:C	1:A:619:LEU:H	2.20	0.45
1:A:1282:PHE:O	1:A:1285:GLU:HG3	2.17	0.45
1:A:1489:THR:HG23	1:A:1491:GLY:H	1.82	0.45
1:A:1386:LYS:HE2	1:A:1386:LYS:HB2	1.66	0.45
2:D:29:SER:O	2:D:33:ILE:HG12	2.17	0.45
1:A:299:TYR:HE1	1:A:307:VAL:H	1.65	0.45
2:D:781:ASN:C	2:D:782:LYS:HG3	2.38	0.44
3:C:58:LYS:NZ	3:C:107:ARG:HE	2.15	0.44
3:C:280:LEU:HD12	3:C:287:PRO:HG2	1.99	0.44
3:C:342:LEU:H	3:C:342:LEU:HD22	1.82	0.44
1:A:691:ASN:HB3	1:A:693:PRO:HD2	1.98	0.44
1:A:1492:GLU:H	1:A:1492:GLU:CD	2.21	0.44
2:D:185:TRP:HA	4:B:1:NAG:H82	1.99	0.44
1:A:929:ARG:O	1:A:953:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:ASP:HB3	1:A:1568:LEU:HD22	1.99	0.44
2:D:575:ARG:O	2:D:579:ILE:HG13	2.17	0.44
2:D:882:LEU:HD21	2:D:1016:ILE:HD13	2.00	0.44
3:C:180:VAL:HA	3:C:288:ILE:HB	1.98	0.44
3:C:203:PHE:HA	3:C:206:HIS:HB2	1.99	0.44
3:C:208:PHE:HA	3:C:211:ARG:HB3	1.99	0.44
2:D:49:LYS:HB3	2:D:49:LYS:HE2	1.67	0.44
2:D:628:PHE:C	2:D:629:TYR:HD1	2.21	0.44
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.87	0.44
1:A:519:ALA:O	1:A:523:SER:HB3	2.17	0.44
1:A:596:VAL:O	1:A:600:ILE:HG13	2.17	0.44
1:A:1012:ASN:O	1:A:1014:VAL:N	2.46	0.44
3:C:212:ILE:HD12	3:C:212:ILE:HA	1.82	0.44
1:A:913:SER:O	1:A:1024:ARG:NH1	2.51	0.44
1:A:1212:TYR:HB3	1:A:1542:LEU:HD11	1.98	0.44
2:D:536:ILE:HD12	2:D:536:ILE:N	2.32	0.44
3:C:330:PRO:C	3:C:332:SER:H	2.18	0.44
1:A:583:TYR:O	1:A:589:ASN:HB3	2.18	0.44
1:A:1482:GLU:O	1:A:1484:GLU:N	2.51	0.44
2:D:108:GLN:NE2	6:F:1:NAG:HN2	2.15	0.44
2:D:254:MET:O	2:D:289:VAL:HA	2.18	0.44
2:D:732:ARG:HD3	2:D:732:ARG:N	2.32	0.44
1:A:1492:GLU:HG2	1:A:1493:THR:N	2.33	0.43
3:C:292:VAL:HA	3:C:337:LEU:HB2	2.00	0.43
3:C:127:ILE:HD12	3:C:130:LYS:HD3	2.00	0.43
1:A:357:PHE:O	1:A:361:THR:HG23	2.17	0.43
1:A:605:LEU:HA	1:A:610:ILE:HD13	1.99	0.43
2:D:378:LYS:HA	2:D:378:LYS:HD2	1.78	0.43
2:D:401:TRP:CZ2	2:D:405:GLU:HG3	2.52	0.43
2:D:596:ASP:OD1	2:D:596:ASP:N	2.45	0.43
3:C:65:ARG:N	3:C:172:ASP:O	2.51	0.43
1:A:428:GLN:HA	1:A:428:GLN:OE1	2.18	0.43
1:A:436:GLY:HA2	3:C:341:GLN:OE1	2.19	0.43
2:D:237:ASP:OD2	2:D:420:ARG:NH1	2.51	0.43
2:D:731:ALA:C	2:D:732:ARG:HD3	2.38	0.43
3:C:44:VAL:O	3:C:47:GLN:HB2	2.18	0.43
3:C:289:ILE:HG22	3:C:333:PHE:HB3	2.00	0.43
2:D:377:ASN:HD21	2:D:406:ASN:HD22	1.66	0.43
3:C:226:ARG:HH21	3:C:254:ILE:HD11	1.82	0.43
3:C:291:PHE:O	3:C:337:LEU:HB2	2.18	0.43
2:D:173:TYR:O	2:D:176:SER:OG	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:GLU:OE1	2:D:210:SER:OG	2.35	0.43
2:D:590:THR:OG1	2:D:591:LEU:N	2.51	0.43
2:D:669:ASP:HB2	2:D:686:PHE:HZ	1.82	0.43
3:C:354:GLU:HA	3:C:354:GLU:OE1	2.18	0.43
1:A:896:ILE:HD13	1:A:970:LEU:HD11	2.01	0.43
3:C:168:VAL:HA	3:C:169:PRO:HD3	1.87	0.43
1:A:1399:TRP:CD1	11:A:2308:PT5:O41	2.72	0.43
3:C:225:LYS:HE3	3:C:282:LYS:HE3	2.00	0.43
3:C:330:PRO:C	3:C:332:SER:N	2.72	0.43
3:C:342:LEU:HA	3:C:345:ALA:HB3	2.01	0.43
3:C:355:VAL:HA	3:C:358:ARG:NH2	2.33	0.43
1:A:298:CYS:HB3	1:A:330:THR:HB	2.00	0.43
2:D:1003:PHE:HB3	2:D:1018:VAL:HG23	2.01	0.43
3:C:95:ILE:HD11	3:C:106:GLY:HA2	2.01	0.43
3:C:186:SER:HB3	3:C:193:THR:HG22	2.01	0.43
1:A:397:LEU:HD23	1:A:1519:PHE:HE2	1.84	0.43
1:A:1062:MET:O	1:A:1066:ILE:HG13	2.18	0.43
1:A:1474:MET:O	1:A:1477:LYS:HE3	2.19	0.43
1:A:1570:ARG:HB3	1:A:1580:LYS:HA	2.01	0.43
3:C:47:GLN:O	3:C:51:GLN:HG2	2.19	0.43
3:C:159:LYS:HD2	3:C:159:LYS:HA	1.77	0.43
2:D:407:LYS:HG2	2:D:1068:TYR:CE1	2.55	0.42
2:D:577:LYS:NZ	2:D:582:GLU:OE1	2.47	0.42
2:D:731:ALA:HB3	2:D:815:LYS:HB2	2.00	0.42
2:D:1030:LEU:H	2:D:1030:LEU:HD23	1.83	0.42
3:C:187:LEU:O	3:C:193:THR:HG21	2.19	0.42
3:C:174:VAL:HG23	3:C:284:SER:O	2.19	0.42
3:C:179:PRO:HA	3:C:266:LEU:O	2.18	0.42
3:C:330:PRO:HG2	3:C:331:GLU:OE2	2.18	0.42
1:A:1017:LEU:HD12	1:A:1020:LEU:HD13	2.01	0.42
1:A:1532:ARG:HD3	1:A:1540:HIS:HD2	1.84	0.42
1:A:1113:ASN:OD1	1:A:1114:SER:N	2.46	0.42
2:D:370:GLN:H	2:D:370:GLN:HG2	1.59	0.42
3:C:179:PRO:O	3:C:288:ILE:N	2.24	0.42
1:A:421:PHE:HE2	1:A:762:LEU:HG	1.85	0.42
1:A:739:CYS:O	1:A:743:ILE:HG13	2.19	0.42
1:A:1537:LEU:HD12	1:A:1541:HIS:HD2	1.85	0.42
3:C:127:ILE:HA	3:C:130:LYS:HB3	2.02	0.42
1:A:380:TRP:H	1:A:381:PRO:HD3	1.85	0.42
1:A:692:PHE:HB3	1:A:693:PRO:HD3	2.01	0.42
1:A:1442:ASN:N	1:A:1445:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1628:GLN:O	1:A:1631:GLU:HG3	2.19	0.42
2:D:241:ARG:HD2	2:D:241:ARG:HA	1.89	0.42
2:D:736:THR:HG23	2:D:810:ALA:HB2	2.01	0.42
3:C:235:ARG:H	3:C:235:ARG:HG2	1.58	0.42
1:A:271:ILE:O	1:A:275:VAL:HG23	2.20	0.42
1:A:441:ILE:HD13	3:C:192:VAL:HG23	2.02	0.42
2:D:203:LEU:HD13	2:D:203:LEU:HA	1.91	0.42
2:D:476:LYS:O	2:D:476:LYS:HG2	2.19	0.42
1:A:573:LEU:O	1:A:577:SER:HB3	2.19	0.42
1:A:965:THR:O	1:A:969:ILE:N	2.39	0.42
1:A:1601:ASP:HB3	1:A:1602:GLY:H	1.62	0.42
2:D:46:THR:O	2:D:50:THR:OG1	2.28	0.42
2:D:97:LEU:HD22	2:D:488:MET:HB3	2.01	0.42
2:D:432:ARG:HB2	2:D:433:PRO:HD3	2.02	0.42
2:D:1002:ILE:HG22	2:D:1019:GLU:OE1	2.19	0.42
3:C:109:VAL:HB	3:C:360:THR:HA	2.02	0.42
1:A:1373:ILE:HD12	1:A:1374:THR:H	1.85	0.41
3:C:63:ALA:CB	3:C:174:VAL:HG12	2.49	0.41
1:A:315:PRO:HG3	1:A:336:TRP:HZ3	1.85	0.41
2:D:67:LEU:HD23	2:D:67:LEU:HA	1.87	0.41
3:C:201:PHE:HA	3:C:204:LEU:HB3	2.02	0.41
2:D:625:THR:O	2:D:626:TYR:CG	2.73	0.41
2:D:656:SER:HA	2:D:716:VAL:HG11	2.01	0.41
3:C:225:LYS:NZ	3:C:279:GLN:O	2.53	0.41
1:A:952:ILE:HD12	1:A:952:ILE:N	2.35	0.41
1:A:1001:LEU:O	1:A:1005:GLY:N	2.53	0.41
2:D:1043:PRO:HA	2:D:1046:MET:HB2	2.02	0.41
3:C:225:LYS:HG2	3:C:282:LYS:HE3	2.01	0.41
1:A:358:GLN:NE2	1:A:713:TYR:OH	2.50	0.41
2:D:377:ASN:HD21	2:D:406:ASN:ND2	2.19	0.41
2:D:449:VAL:HG12	2:D:458:LEU:HD22	2.02	0.41
2:D:1039:ASP:OD1	2:D:1039:ASP:N	2.53	0.41
1:A:440:TRP:HD1	1:A:440:TRP:O	2.04	0.41
1:A:633:TYR:N	1:A:633:TYR:CD1	2.87	0.41
1:A:1129:PHE:O	1:A:1133:THR:HG23	2.20	0.41
1:A:434:LEU:O	1:A:438:LEU:HB3	2.21	0.41
2:D:780:PHE:CD2	2:D:781:ASN:N	2.89	0.41
2:D:894:PHE:HE2	2:D:896:LYS:HE2	1.85	0.41
3:C:340:ASN:HB3	3:C:341:GLN:H	1.74	0.41
1:A:126:PHE:O	1:A:130:ILE:HG13	2.21	0.41
1:A:152:SER:HB3	2:D:330:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD11	1:A:207:LEU:HD12	2.01	0.41
1:A:271:ILE:HD11	1:A:403:VAL:HG21	2.02	0.41
1:A:923:VAL:HB	1:A:1482:GLU:CG	2.51	0.41
1:A:1474:MET:O	1:A:1496:GLY:HA3	2.21	0.41
2:D:322:VAL:O	2:D:325:ILE:HG12	2.21	0.41
2:D:672:ILE:HA	2:D:679:PHE:CE2	2.55	0.41
2:D:763:PHE:O	2:D:767:SER:OG	2.31	0.41
3:C:77:GLU:HB3	3:C:103:TRP:CZ2	2.55	0.41
1:A:1570:ARG:HD2	1:A:1570:ARG:N	2.30	0.41
3:C:265:GLN:O	3:C:267:VAL:HG23	2.21	0.41
1:A:158:ASN:O	1:A:162:VAL:HG23	2.22	0.40
3:C:240:ARG:NE	3:C:242:SER:OG	2.54	0.40
1:A:1172:ILE:O	1:A:1176:PHE:HB3	2.21	0.40
3:C:180:VAL:HB	3:C:268:VAL:HA	2.03	0.40
1:A:124:LYS:CB	1:A:125:PRO:HD3	2.46	0.40
2:D:66:ASP:O	2:D:634:LYS:HE3	2.22	0.40
2:D:130:ASP:OD1	2:D:130:ASP:N	2.53	0.40
2:D:232:LYS:HA	2:D:232:LYS:HD3	1.68	0.40
2:D:289:VAL:HG12	2:D:310:ALA:HB2	2.03	0.40
2:D:704:ARG:HH11	2:D:704:ARG:HG2	1.86	0.40
3:C:236:THR:HG23	3:C:237:ILE:HG13	2.03	0.40
2:D:735:VAL:HB	2:D:811:VAL:HG12	2.03	0.40
2:D:772:ASN:HB2	2:D:1010:ASN:O	2.21	0.40
2:D:852:ILE:HG23	2:D:1015:PHE:HD1	1.85	0.40
3:C:235:ARG:HB2	3:C:238:ILE:HB	2.03	0.40
3:C:264:LEU:HD22	3:C:264:LEU:HA	1.94	0.40
1:A:1036:LYS:HZ2	1:A:1036:LYS:HG3	1.79	0.40
9:A:2303:CLR:H162	9:A:2303:CLR:H221	1.50	0.40
9:A:2304:CLR:H221	9:A:2304:CLR:H162	1.25	0.40
2:D:264:VAL:O	2:D:268:THR:HG23	2.22	0.40
2:D:884:ARG:NH2	2:D:1029:ARG:HG2	2.36	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	1244/2201 (56%)	1152 (93%)	85 (7%)	7 (1%)	22	52
2	D	936/1103 (85%)	883 (94%)	53 (6%)	0	100	100
3	C	322/484 (66%)	244 (76%)	72 (22%)	6 (2%)	6	24
All	All	2502/3788 (66%)	2279 (91%)	210 (8%)	13 (0%)	27	56

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	140	ASN
3	C	310	SER
3	C	330	PRO
1	A	124	LYS
1	A	622	VAL
1	A	233	VAL
3	C	136	ARG
3	C	315	LEU
1	A	1481	PRO
1	A	1493	THR
3	C	267	VAL
1	A	1557	LYS
1	A	1294	LYS

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	1117/1896 (59%)	1023 (92%)	94 (8%)	9	28
2	D	837/971 (86%)	772 (92%)	65 (8%)	10	31
3	C	287/426 (67%)	238 (83%)	49 (17%)	1	5
All	All	2241/3293 (68%)	2033 (91%)	208 (9%)	10	23

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	PHE
1	A	137	ASN
1	A	171	THR
1	A	208	PHE
1	A	234	LYS
1	A	236	LEU
1	A	242	LEU
1	A	249	SER
1	A	253	SER
1	A	293	LYS
1	A	299	TYR
1	A	306	ASP
1	A	332	CYS
1	A	348	ASN
1	A	358	GLN
1	A	360	ILE
1	A	409	SER
1	A	412	ARG
1	A	439	ASP
1	A	445	GLU
1	A	508	ARG
1	A	512	PHE
1	A	513	CYS
1	A	541	ILE
1	A	557	ASP
1	A	576	TYR
1	A	587	LEU
1	A	602	GLU
1	A	611	MET
1	A	622	VAL
1	A	635	ASN
1	A	636	SER
1	A	647	SER
1	A	649	ARG
1	A	656	LEU
1	A	682	MET
1	A	685	ARG
1	A	686	ARG
1	A	698	THR
1	A	746	ASN
1	A	780	ARG
1	A	907	LEU
1	A	909	PHE

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Mol	Chain	Res	Type
1	A	925	HIS
1	A	927	SER
1	A	928	PHE
1	A	957	ASP
1	A	959	VAL
1	A	961	THR
1	A	965	THR
1	A	968	ILE
1	A	975	TYR
1	A	986	ARG
1	A	988	TYR
1	A	1000	SER
1	A	1015	LYS
1	A	1016	ILE
1	A	1051	ASN
1	A	1081	SER
1	A	1082	SER
1	A	1084	GLN
1	A	1094	ILE
1	A	1097	LYS
1	A	1120	ASN
1	A	1178	MET
1	A	1217	ARG
1	A	1238	SER
1	A	1243	TYR
1	A	1258	MET
1	A	1264	SER
1	A	1268	LYS
1	A	1285	GLU
1	A	1288	LEU
1	A	1296	LYS
1	A	1304	ASN
1	A	1314	SER
1	A	1401	PHE
1	A	1408	LEU
1	A	1428	GLN
1	A	1442	ASN
1	A	1449	THR
1	A	1493	THR
1	A	1495	CYS
1	A	1515	ILE
1	A	1540	HIS

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Mol	Chain	Res	Type
1	A	1549	TRP
1	A	1562	HIS
1	A	1570	ARG
1	A	1572	ILE
1	A	1585	ARG
1	A	1599	ASN
1	A	1601	ASP
1	A	1605	MET
1	A	1646	MET
2	D	34	LYS
2	D	39	LYS
2	D	54	VAL
2	D	64	TYR
2	D	89	LEU
2	D	128	LYS
2	D	130	ASP
2	D	139	GLU
2	D	154	ASN
2	D	176	SER
2	D	203	LEU
2	D	246	GLN
2	D	268	THR
2	D	279	MET
2	D	284	SER
2	D	359	MET
2	D	367	GLU
2	D	375	LYS
2	D	406	ASN
2	D	416	ILE
2	D	428	ASP
2	D	463	THR
2	D	476	LYS
2	D	477	THR
2	D	506	LEU
2	D	507	CYS
2	D	516	ASP
2	D	538	THR
2	D	553	SER
2	D	555	GLU
2	D	587	THR
2	D	590	THR
2	D	602	LYS

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Mol	Chain	Res	Type
2	D	615	THR
2	D	634	LYS
2	D	643	ARG
2	D	655	GLU
2	D	665	ASP
2	D	685	GLU
2	D	686	PHE
2	D	693	ASN
2	D	701	LEU
2	D	732	ARG
2	D	764	TYR
2	D	766	ARG
2	D	770	ASN
2	D	780	PHE
2	D	782	LYS
2	D	788	TYR
2	D	795	SER
2	D	798	VAL
2	D	827	LYS
2	D	845	SER
2	D	848	MET
2	D	849	ASP
2	D	850	CYS
2	D	877	GLU
2	D	883	MET
2	D	973	SER
2	D	979	THR
2	D	984	ASP
2	D	989	SER
2	D	991	SER
2	D	1003	PHE
2	D	1029	ARG
3	C	41	ARG
3	C	42	ARG
3	C	46	SER
3	C	51	GLN
3	C	52	LEU
3	C	80	VAL
3	C	83	SER
3	C	93	LEU
3	C	94	HIS
3	C	95	ILE

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Mol	Chain	Res	Type
3	C	96	LYS
3	C	108	LEU
3	C	110	LYS
3	C	114	ASP
3	C	120	SER
3	C	122	GLN
3	C	126	SER
3	C	129	LEU
3	C	134	LYS
3	C	149	ASN
3	C	152	SER
3	C	163	LYS
3	C	168	VAL
3	C	191	GLU
3	C	194	ASP
3	C	205	LYS
3	C	206	HIS
3	C	211	ARG
3	C	225	LYS
3	C	226	ARG
3	C	227	SER
3	C	235	ARG
3	C	262	LYS
3	C	263	SER
3	C	264	LEU
3	C	265	GLN
3	C	266	LEU
3	C	269	LEU
3	C	282	LYS
3	C	284	SER
3	C	296	SER
3	C	306	SER
3	C	307	ARG
3	C	312	MET
3	C	322	TYR
3	C	324	LYS
3	C	325	LEU
3	C	327	GLN
3	C	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	537	ASN
2	D	314	ASN
2	D	684	ASN
3	C	265	GLN

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](#)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1	2,4	14,14,15	0.81	1 (7%)	17,19,21	1.18	1 (5%)
4	NAG	B	2	4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	B	3	4	14,14,15	0.31	0	17,19,21	0.40	0
5	NAG	E	1	2,5	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	E	2	5	14,14,15	0.59	0	17,19,21	0.79	0
6	NAG	F	1	2,6	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	F	3	6	14,14,15	1.01	1 (7%)	17,19,21	1.69	2 (11%)
6	NAG	F	4	6	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
5	NAG	G	1	2,5	14,14,15	0.35	0	17,19,21	0.42	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.48	0
5	NAG	H	1	2,5	14,14,15	0.48	0	17,19,21	0.39	0
5	NAG	H	2	5	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
4	NAG	B	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	NAG	B	3	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	5/6/23/26	0/1/1/1
6	NAG	F	4	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.38	1.49	1.43
4	B	1	NAG	O5-C1	2.80	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	NAG	C1-O5-C5	4.68	118.53	112.19
4	B	1	NAG	C1-O5-C5	4.59	118.41	112.19
6	F	3	NAG	C2-N2-C7	4.38	129.13	122.90
6	F	4	NAG	C2-N2-C7	4.30	129.03	122.90
6	F	4	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	3	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6

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

There are no ring outliers.

7 monomers are involved in 9 short contacts:

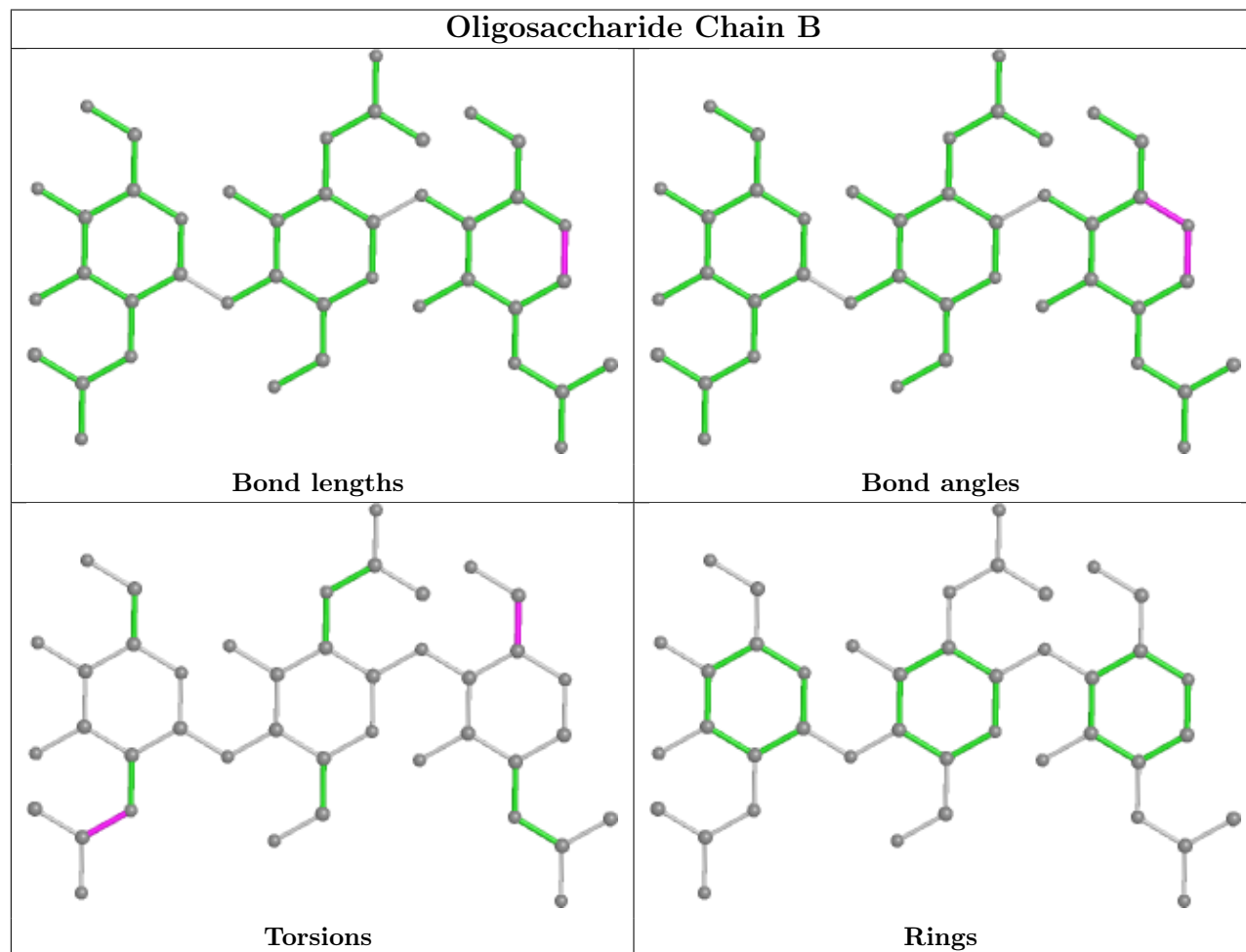
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3	NAG	2	0
6	F	4	NAG	1	0
4	B	1	NAG	3	0
5	G	1	NAG	1	0
5	H	1	NAG	1	0

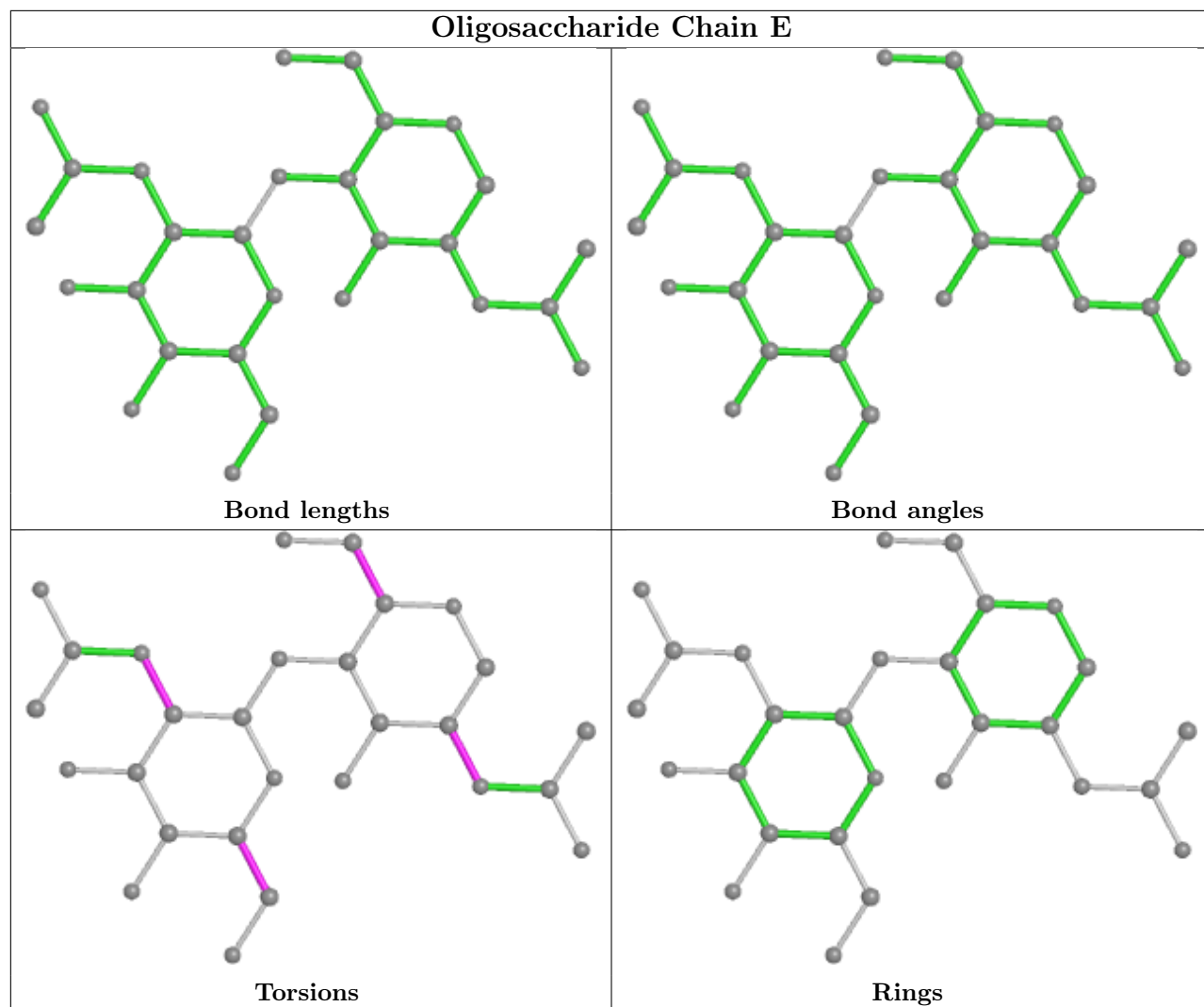
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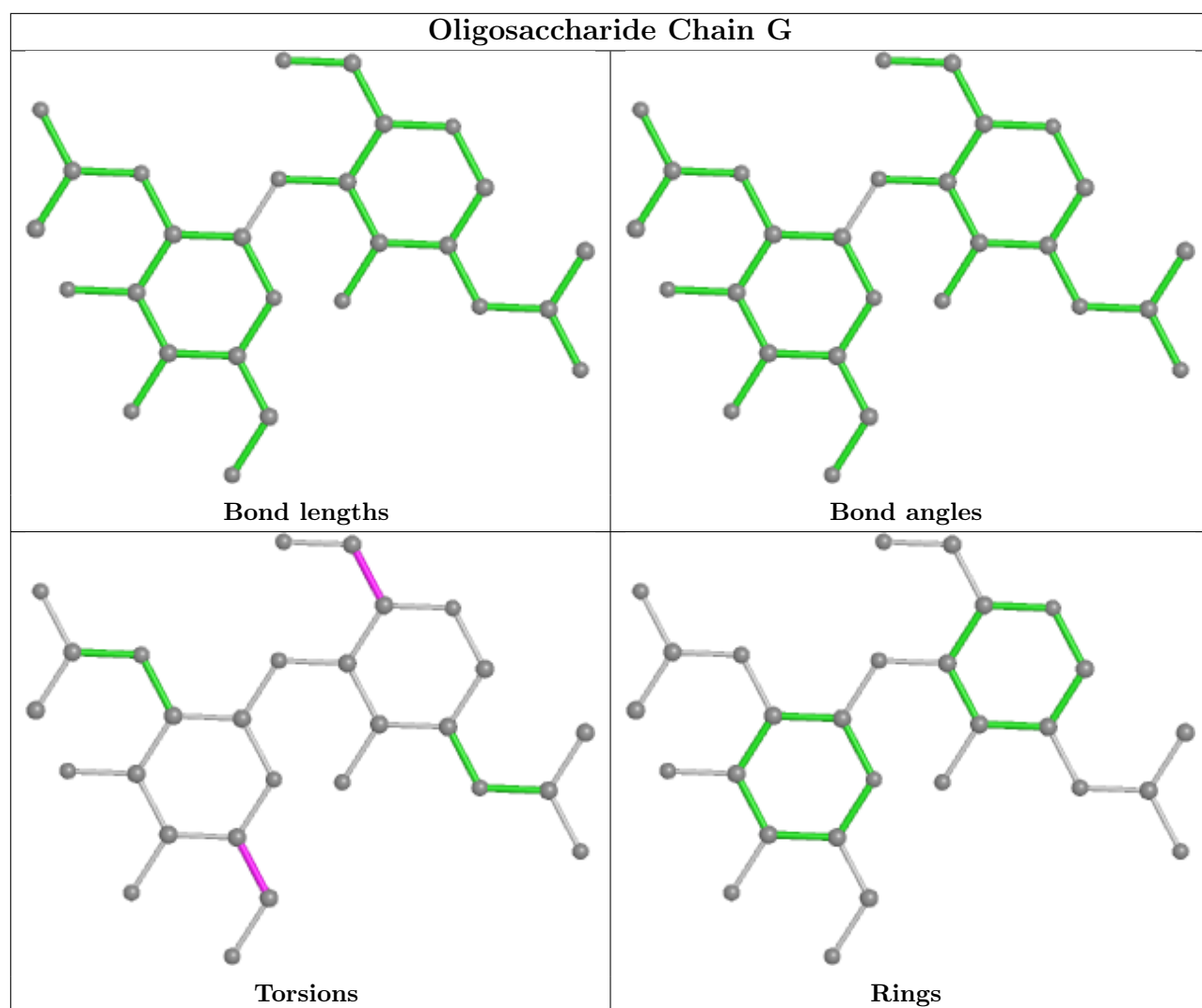
Continued from previous page...

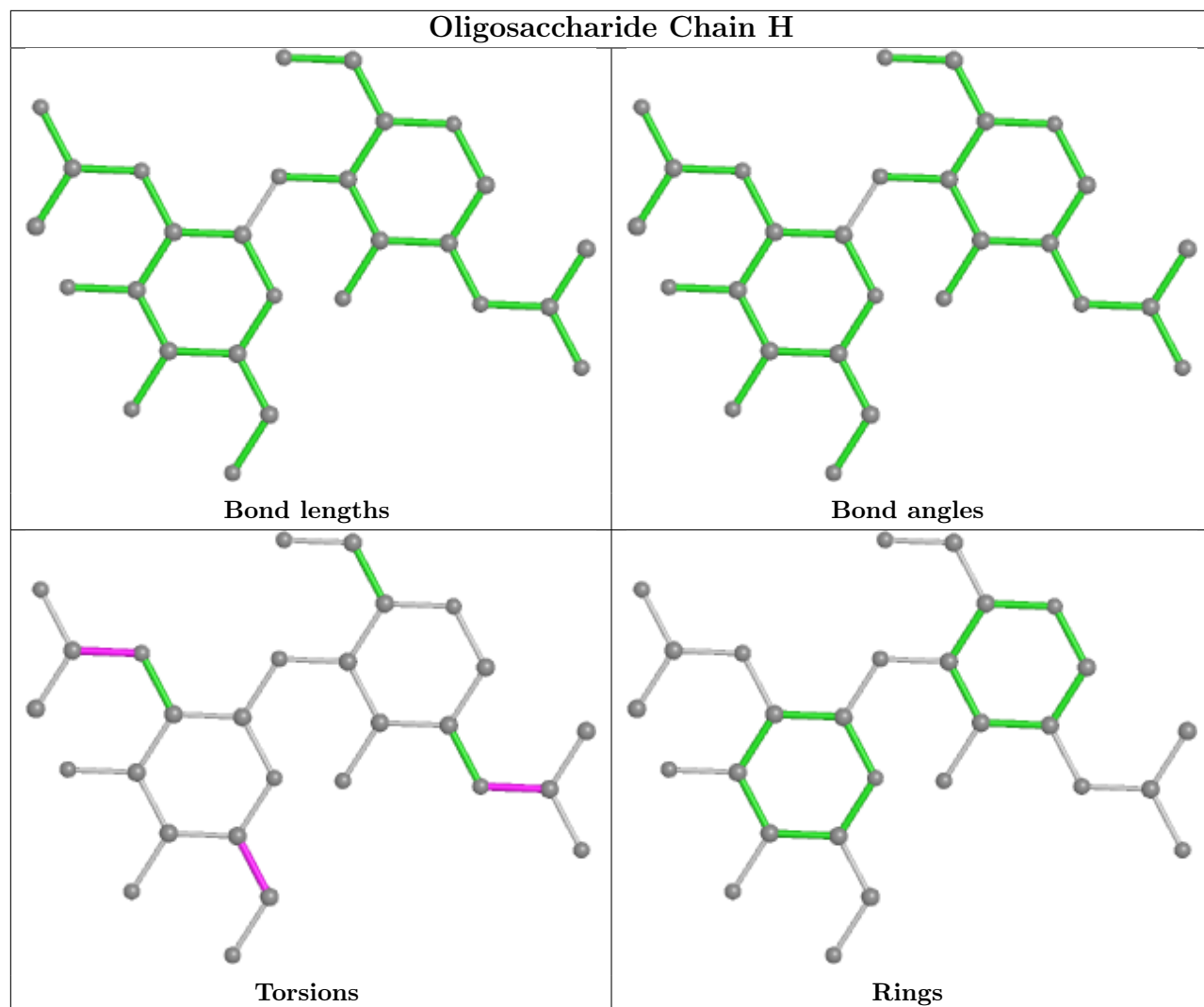
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0
5	G	2	NAG	1	0

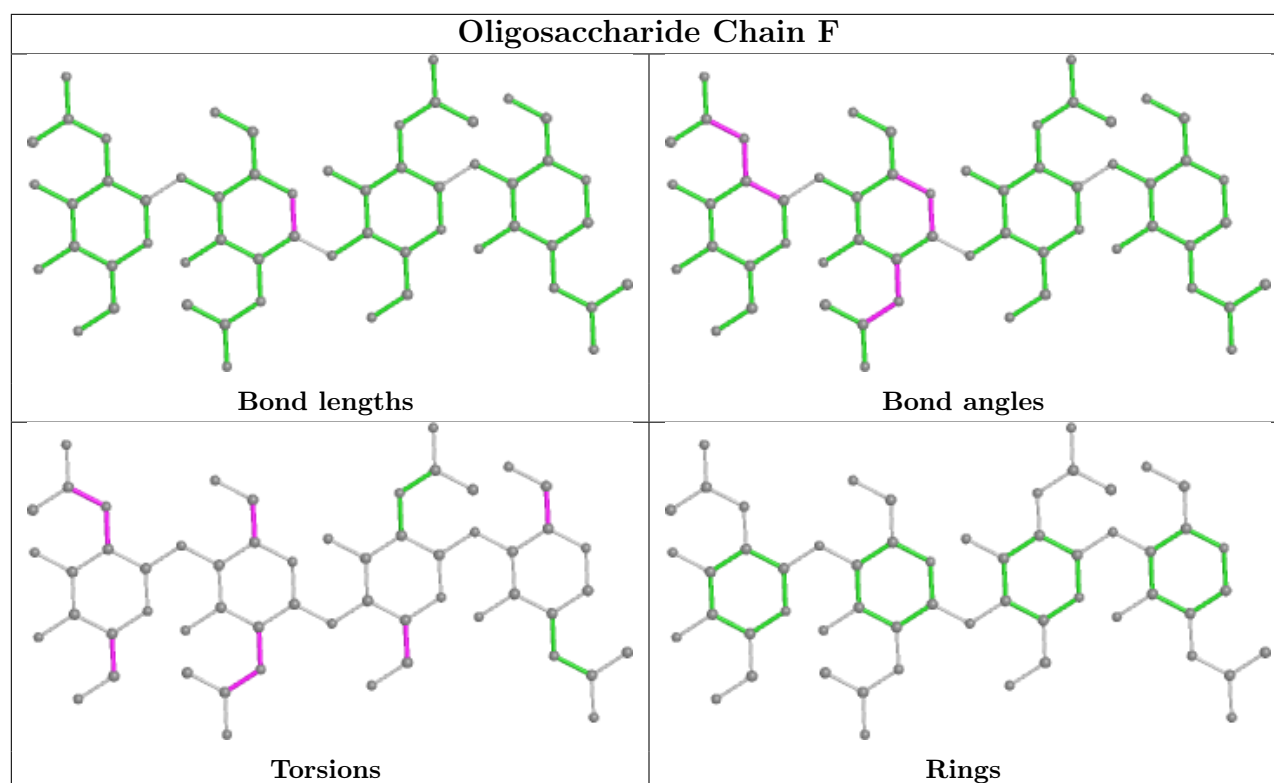
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
9	CLR	A	2306	-	31,31,31	0.38	0	48,48,48	0.70	1 (2%)
9	CLR	A	2305	-	31,31,31	0.35	0	48,48,48	0.50	0
10	NAG	A	2307	1	14,14,15	0.42	0	17,19,21	1.27	1 (5%)
11	PT5	A	2308	-	63,63,69	0.86	2 (3%)	76,81,87	1.04	4 (5%)
10	NAG	D	1202	2	14,14,15	0.48	0	17,19,21	0.43	0
10	NAG	D	1203	2	14,14,15	0.83	1 (7%)	17,19,21	0.99	1 (5%)
9	CLR	A	2304	-	31,31,31	0.40	0	48,48,48	0.84	1 (2%)
9	CLR	A	2303	-	31,31,31	0.39	0	48,48,48	0.68	0
8	3PE	A	2302	-	39,39,50	0.57	0	42,44,55	0.62	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLR	A	2306	-	-	10/10/68/68	0/4/4/4
9	CLR	A	2305	-	-	6/10/68/68	0/4/4/4
10	NAG	A	2307	1	-	2/6/23/26	0/1/1/1
11	PT5	A	2308	-	-	20/60/84/90	0/1/1/1
10	NAG	D	1202	2	-	2/6/23/26	0/1/1/1
10	NAG	D	1203	2	-	2/6/23/26	0/1/1/1
9	CLR	A	2304	-	-	6/10/68/68	0/4/4/4
9	CLR	A	2303	-	-	6/10/68/68	0/4/4/4
8	3PE	A	2302	-	-	14/43/43/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2308	PT5	O18-C11	3.98	1.45	1.33
11	A	2308	PT5	O16-C10	3.88	1.45	1.34
10	D	1203	NAG	O5-C1	2.77	1.48	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2307	NAG	C1-O5-C5	4.75	118.63	112.19
10	D	1203	NAG	C1-O5-C5	3.82	117.37	112.19
11	A	2308	PT5	O16-C10-C12	3.41	118.86	111.50
11	A	2308	PT5	O18-C11-C31	3.29	122.22	111.91
11	A	2308	PT5	O18-C11-O19	-2.88	116.33	123.59
9	A	2304	CLR	C1-C2-C3	2.43	113.58	110.47
8	A	2302	3PE	O12-P-O14	2.36	123.91	112.24
11	A	2308	PT5	C5-C6-C1	2.13	113.37	108.96
9	A	2306	CLR	C16-C15-C14	-2.03	101.11	105.13

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2302	3PE	C1-O11-P-O14
8	A	2302	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
8	A	2302	3PE	C11-O13-P-O12
8	A	2302	3PE	C11-O13-P-O14
9	A	2304	CLR	C13-C17-C20-C21
9	A	2304	CLR	C13-C17-C20-C22
9	A	2304	CLR	C16-C17-C20-C21
11	A	2308	PT5	C7-O13-P1-O12
11	A	2308	PT5	C7-O13-P1-O11
11	A	2308	PT5	C7-O13-P1-O1
11	A	2308	PT5	C6-C1-O1-P1
11	A	2308	PT5	C2-C1-O1-P1
11	A	2308	PT5	C19-C20-C21-C22
9	A	2304	CLR	C16-C17-C20-C22
9	A	2303	CLR	C21-C20-C22-C23
9	A	2304	CLR	C21-C20-C22-C23
9	A	2305	CLR	C16-C17-C20-C21
9	A	2305	CLR	C13-C17-C20-C21
9	A	2303	CLR	C13-C17-C20-C22
9	A	2305	CLR	C13-C17-C20-C22
8	A	2302	3PE	C32-C31-O31-C3
10	A	2307	NAG	C4-C5-C6-O6
8	A	2302	3PE	O32-C31-O31-C3
9	A	2305	CLR	C16-C17-C20-C22
10	D	1203	NAG	O5-C5-C6-O6
9	A	2303	CLR	C16-C17-C20-C21
9	A	2303	CLR	C13-C17-C20-C21
9	A	2304	CLR	C17-C20-C22-C23
9	A	2306	CLR	C21-C20-C22-C23
10	A	2307	NAG	O5-C5-C6-O6
9	A	2303	CLR	C16-C17-C20-C22
9	A	2305	CLR	C17-C20-C22-C23
9	A	2306	CLR	C17-C20-C22-C23
9	A	2305	CLR	C21-C20-C22-C23
10	D	1202	NAG	C8-C7-N2-C2
10	D	1202	NAG	O7-C7-N2-C2
9	A	2303	CLR	C17-C20-C22-C23
10	D	1203	NAG	C4-C5-C6-O6
9	A	2306	CLR	C13-C17-C20-C22
8	A	2302	3PE	C35-C36-C37-C38
8	A	2302	3PE	C26-C27-C28-C29
11	A	2308	PT5	C34-C35-C36-C37
11	A	2308	PT5	C35-C36-C37-C38
11	A	2308	PT5	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
11	A	2308	PT5	C10-C12-C13-C14
9	A	2306	CLR	C16-C17-C20-C21
9	A	2306	CLR	C13-C17-C20-C21
9	A	2306	CLR	C16-C17-C20-C22
8	A	2302	3PE	C22-C21-O21-C2
8	A	2302	3PE	O22-C21-O21-C2
8	A	2302	3PE	O11-C1-C2-C3
11	A	2308	PT5	C38-C39-C40-C41
9	A	2306	CLR	C22-C23-C24-C25
11	A	2308	PT5	O13-C7-C8-O16
11	A	2308	PT5	O13-C7-C8-C9
11	A	2308	PT5	C1-O1-P1-O13
8	A	2302	3PE	C1-O11-P-O13
11	A	2308	PT5	C21-C22-C23-C24
9	A	2306	CLR	C23-C24-C25-C27
8	A	2302	3PE	C1-C2-O21-C21
8	A	2302	3PE	O11-C1-C2-O21
11	A	2308	PT5	C13-C14-C15-C16
9	A	2306	CLR	C23-C24-C25-C26
11	A	2308	PT5	C1-O1-P1-O12
11	A	2308	PT5	C9-C8-O16-C10
11	A	2308	PT5	C18-C19-C20-C21
11	A	2308	PT5	C37-C38-C39-C40
9	A	2306	CLR	C20-C22-C23-C24

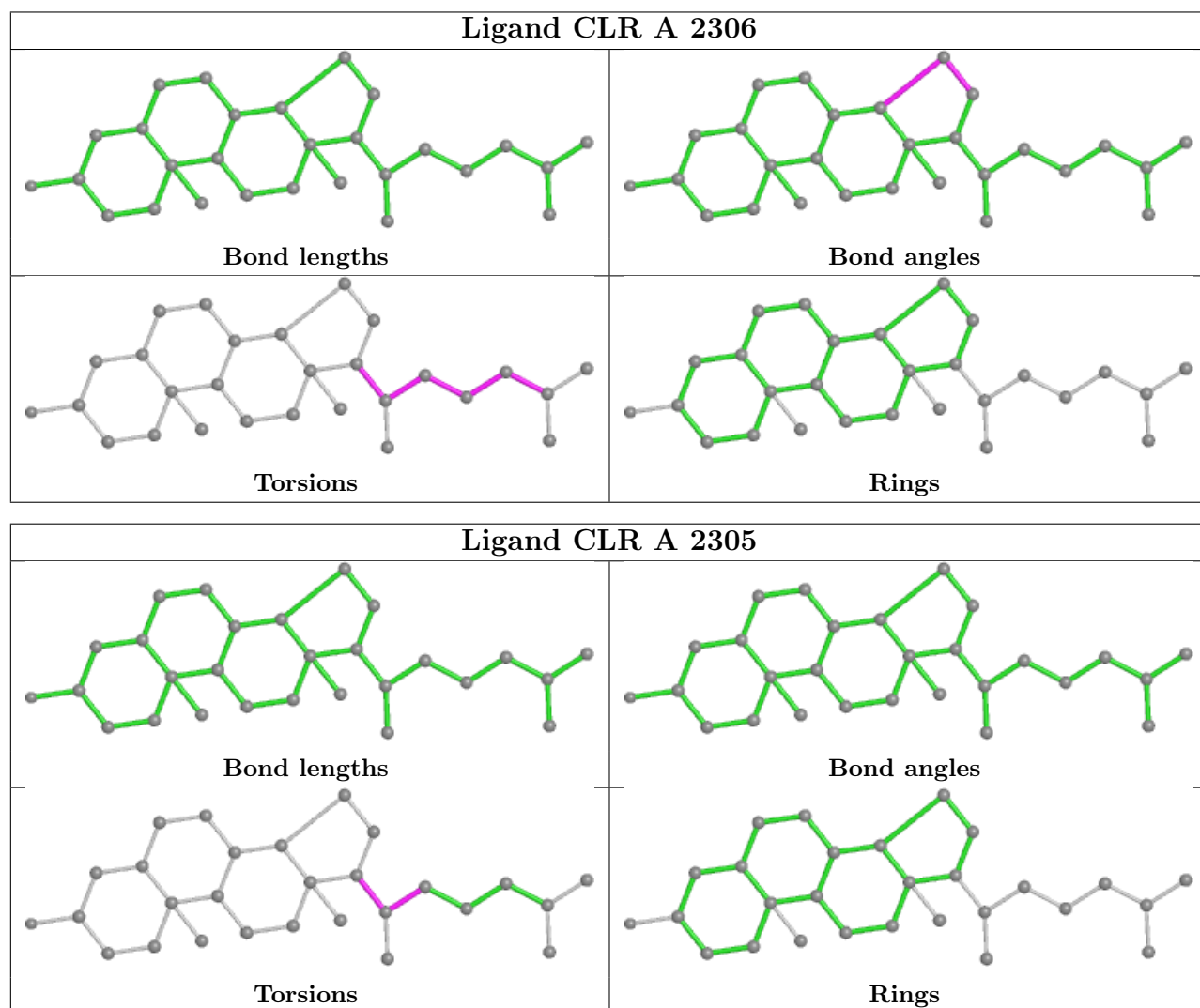
There are no ring outliers.

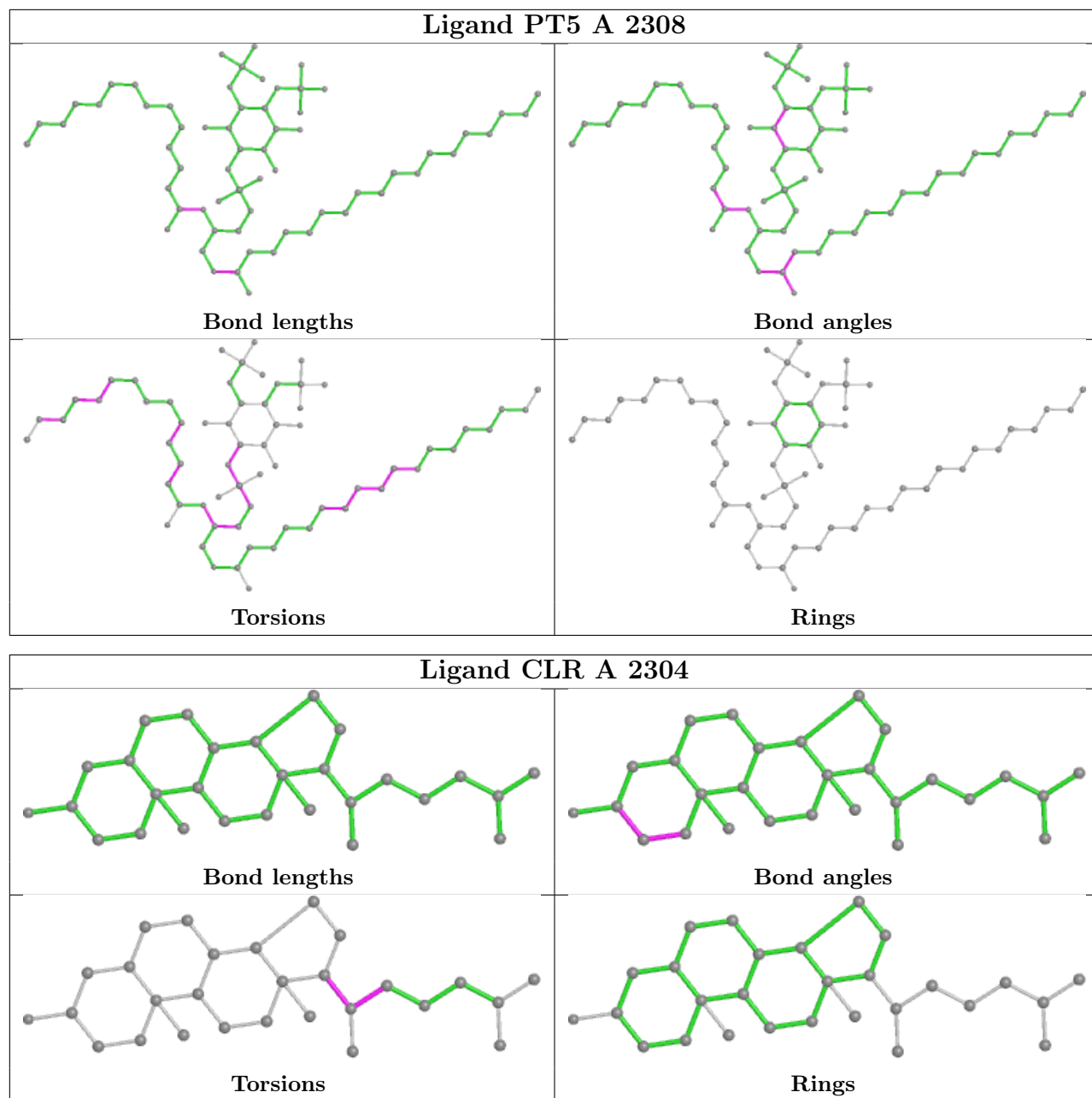
6 monomers are involved in 10 short contacts:

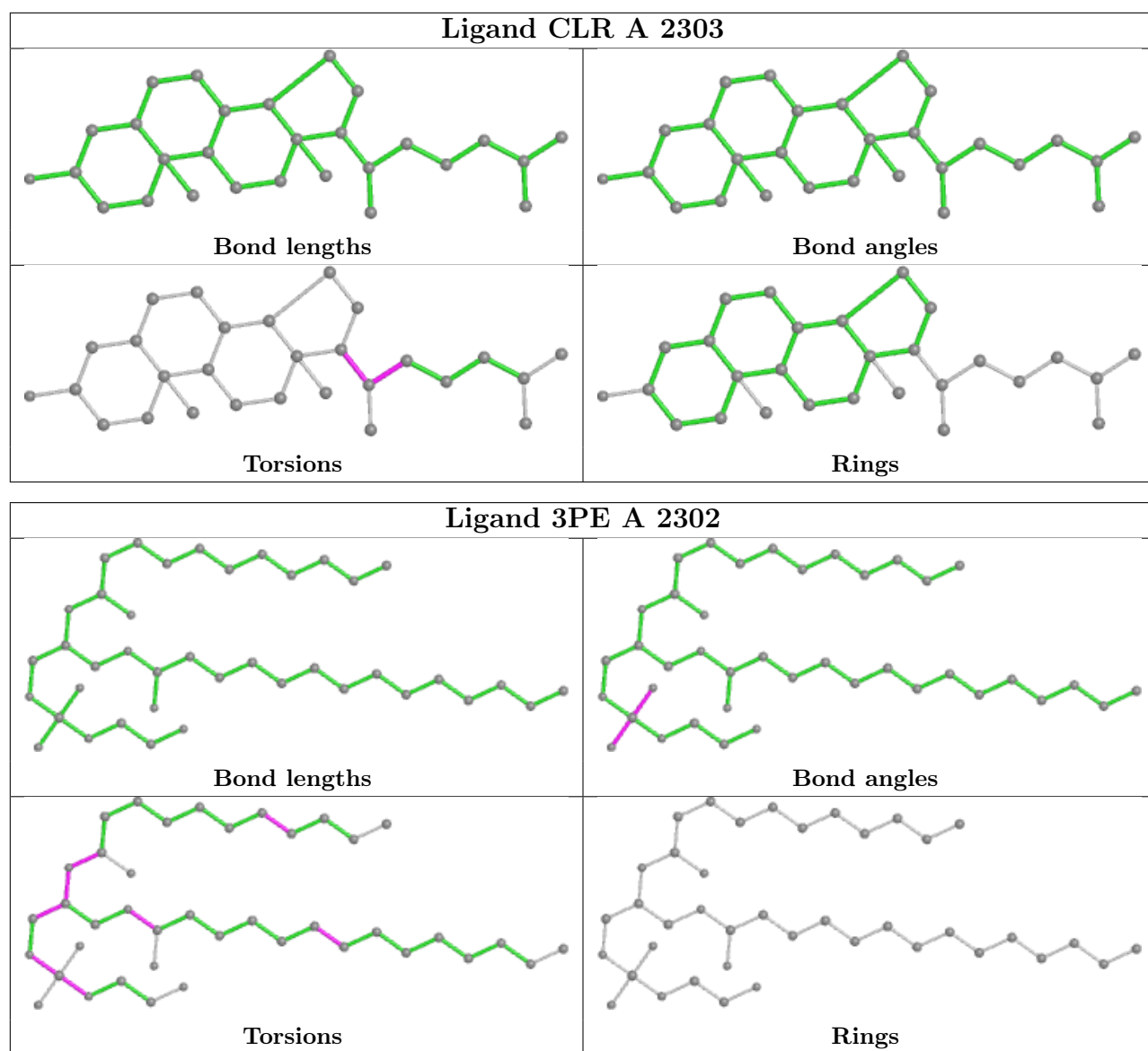
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2306	CLR	2	0
9	A	2305	CLR	1	0
11	A	2308	PT5	1	0
9	A	2304	CLR	3	0
9	A	2303	CLR	2	0
8	A	2302	3PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

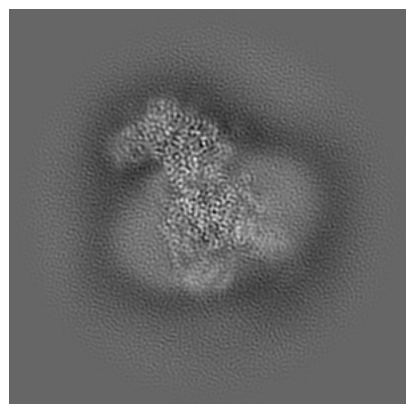
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37472. These allow visual inspection of the internal detail of the map and identification of artifacts.

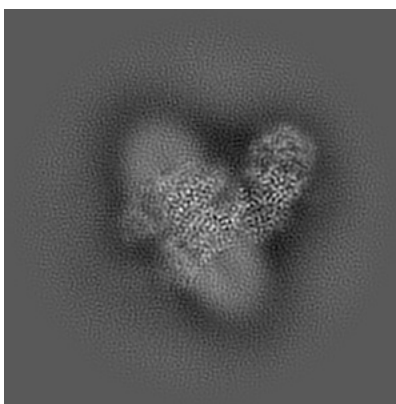
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

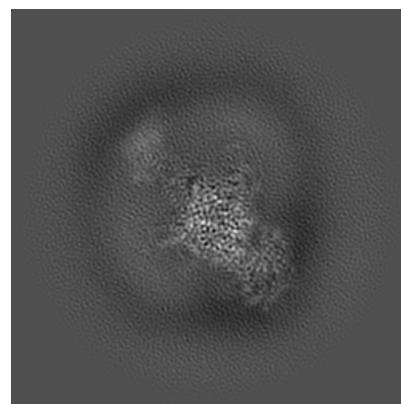
6.1.1 Primary map



X

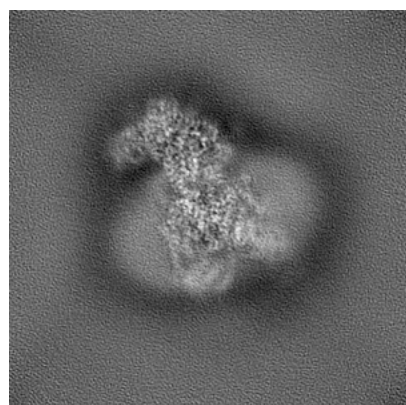


Y

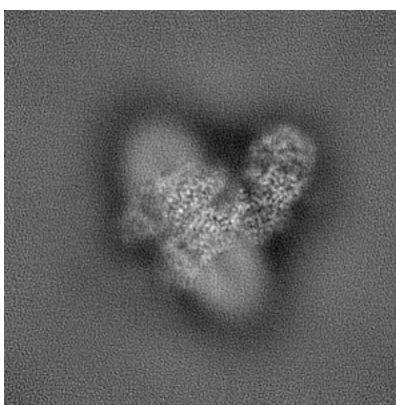


Z

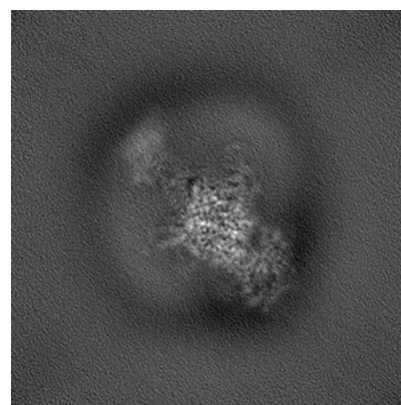
6.1.2 Raw map



X



Y

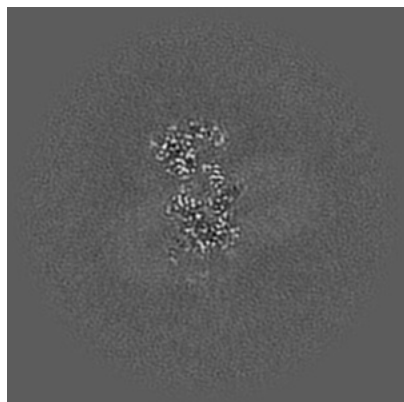


Z

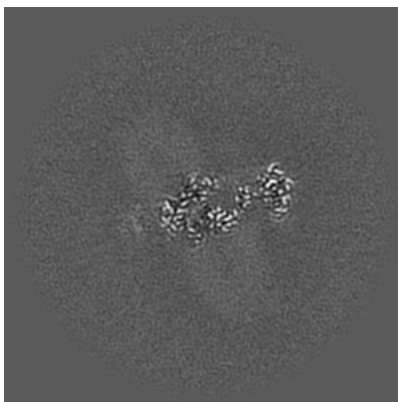
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

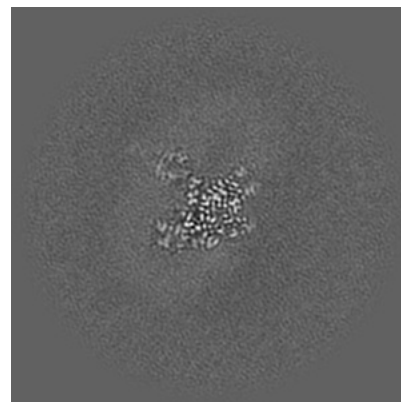
6.2.1 Primary map



X Index: 140

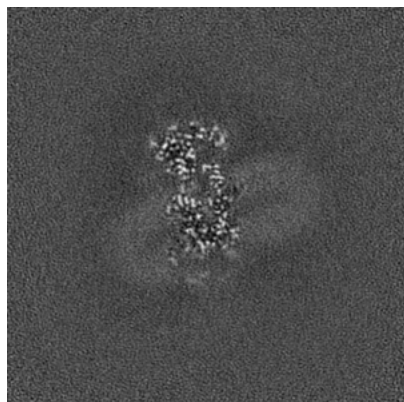


Y Index: 140

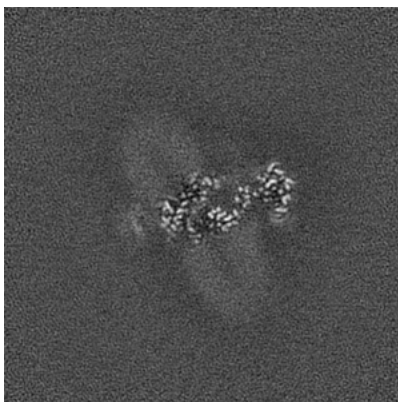


Z Index: 140

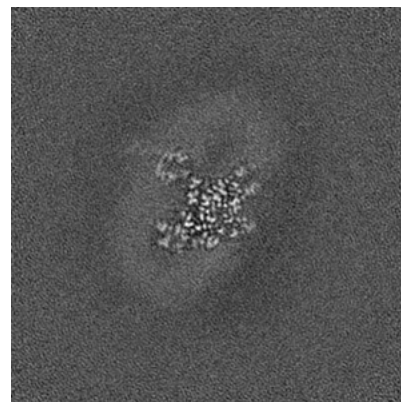
6.2.2 Raw map



X Index: 140



Y Index: 140

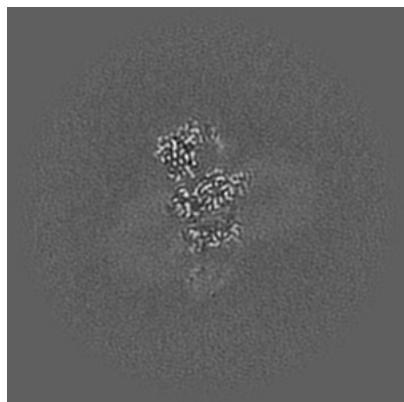


Z Index: 140

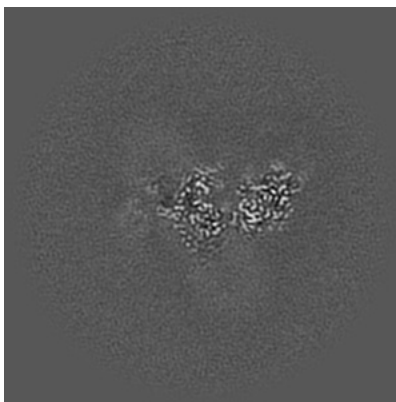
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

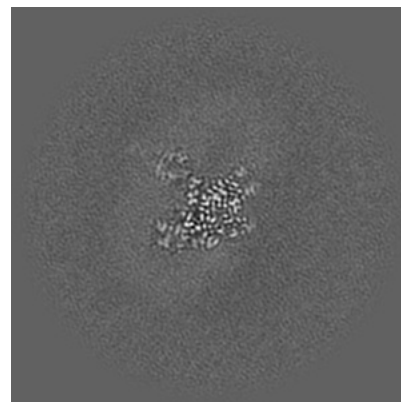
6.3.1 Primary map



X Index: 135

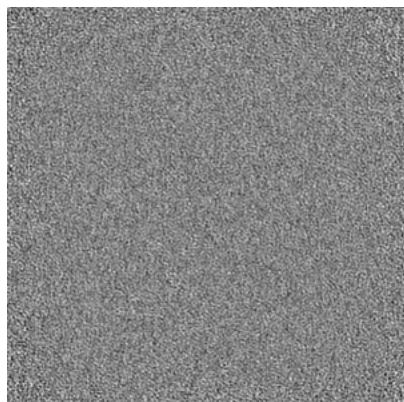


Y Index: 130

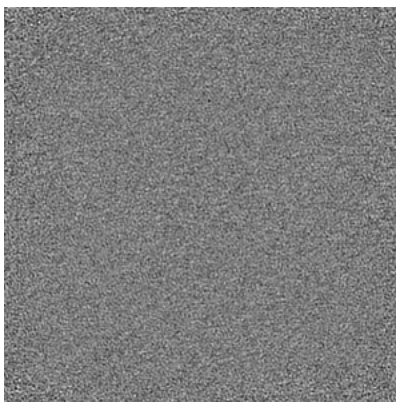


Z Index: 140

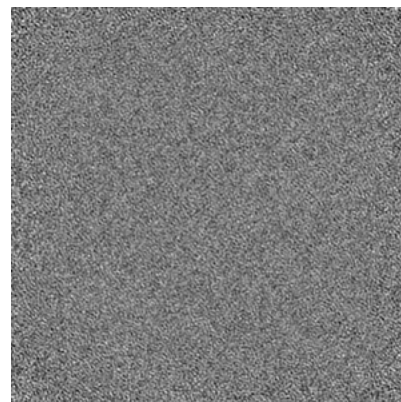
6.3.2 Raw map



X Index: 0



Y Index: 0

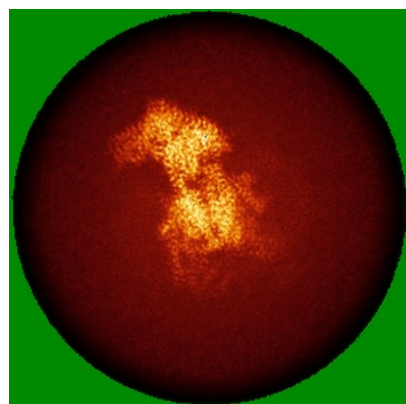


Z Index: 0

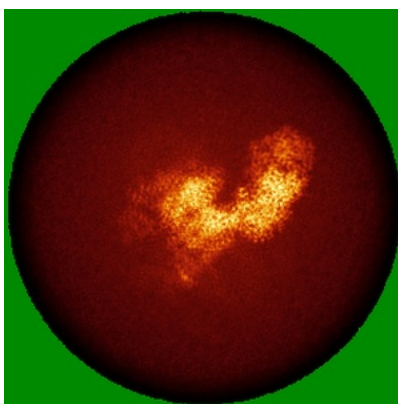
The images above show the largest variance slices of the map in three orthogonal directions.

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

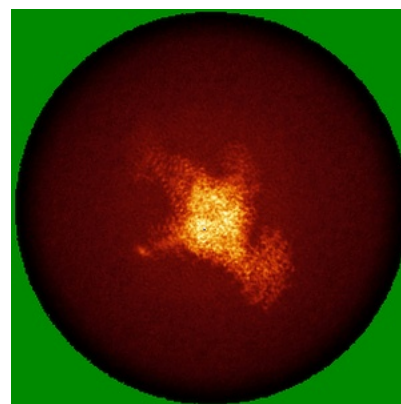
6.4.1 Primary map



X

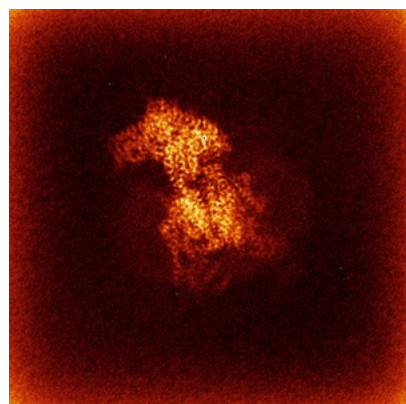


Y

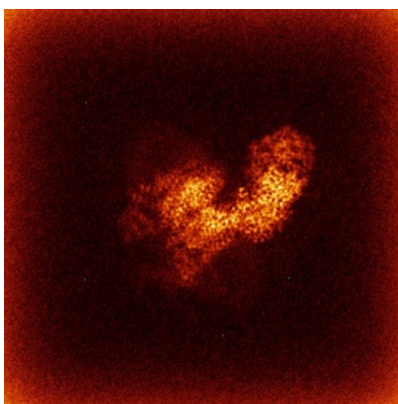


Z

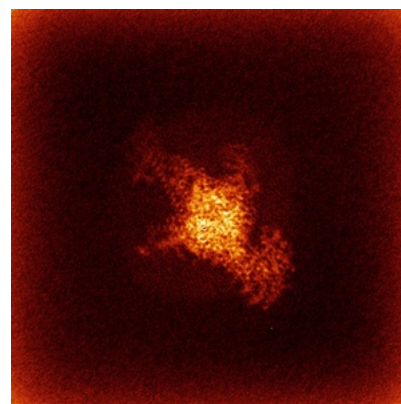
6.4.2 Raw map



X



Y

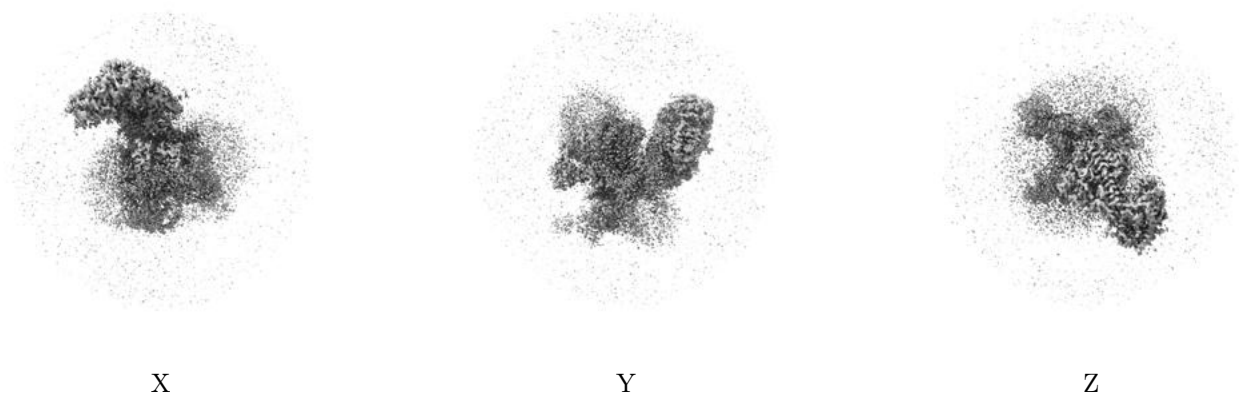


Z

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.

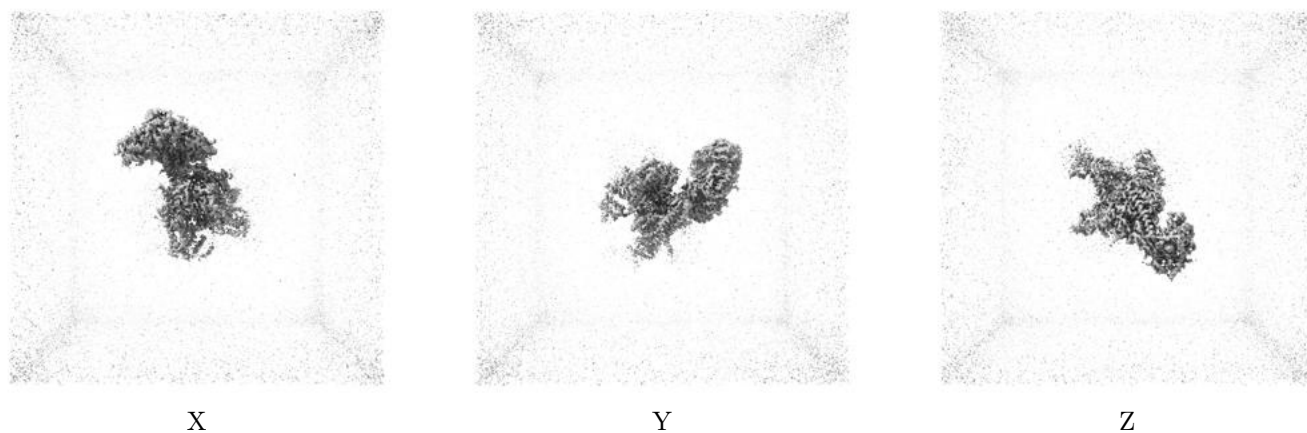
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

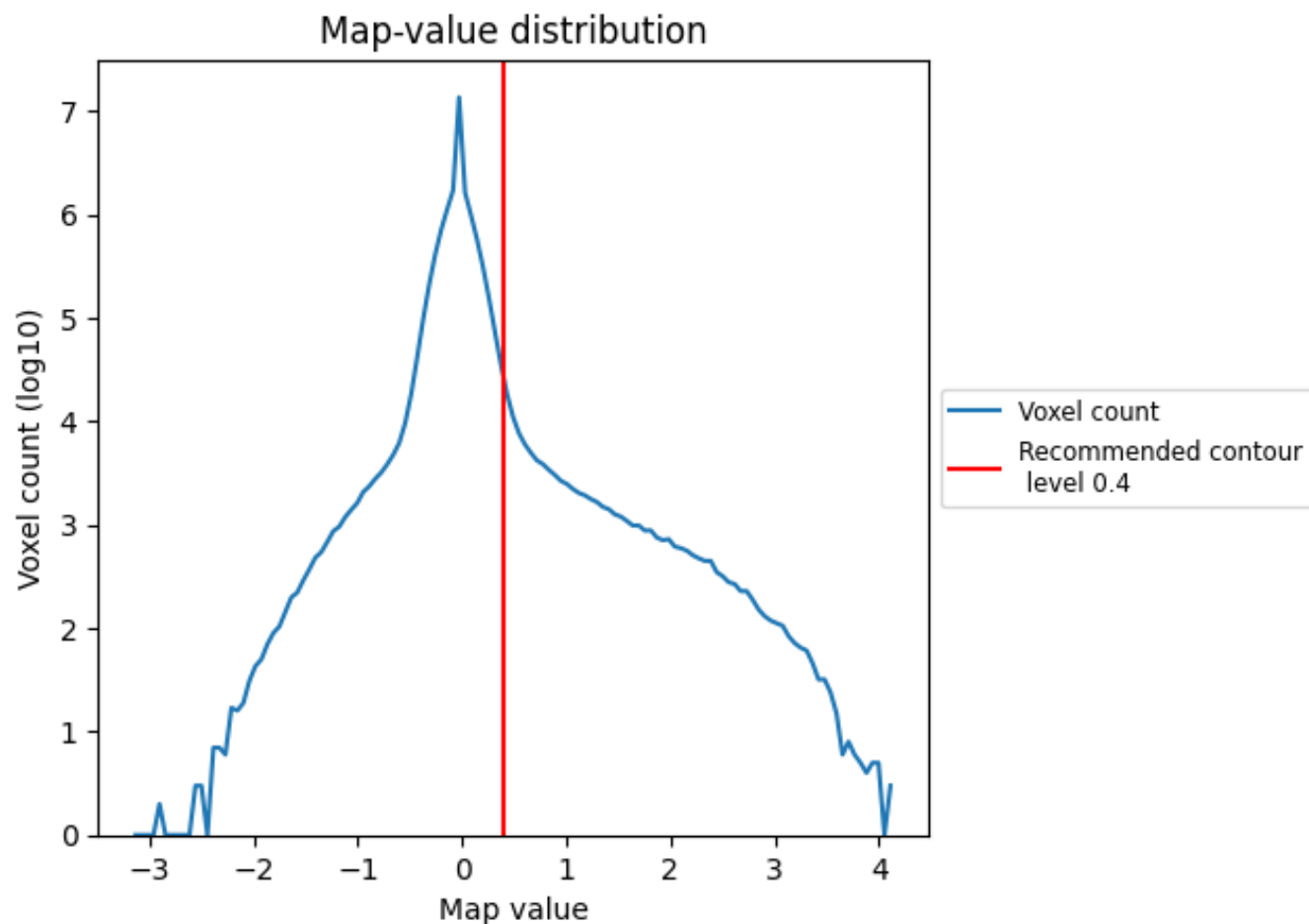
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

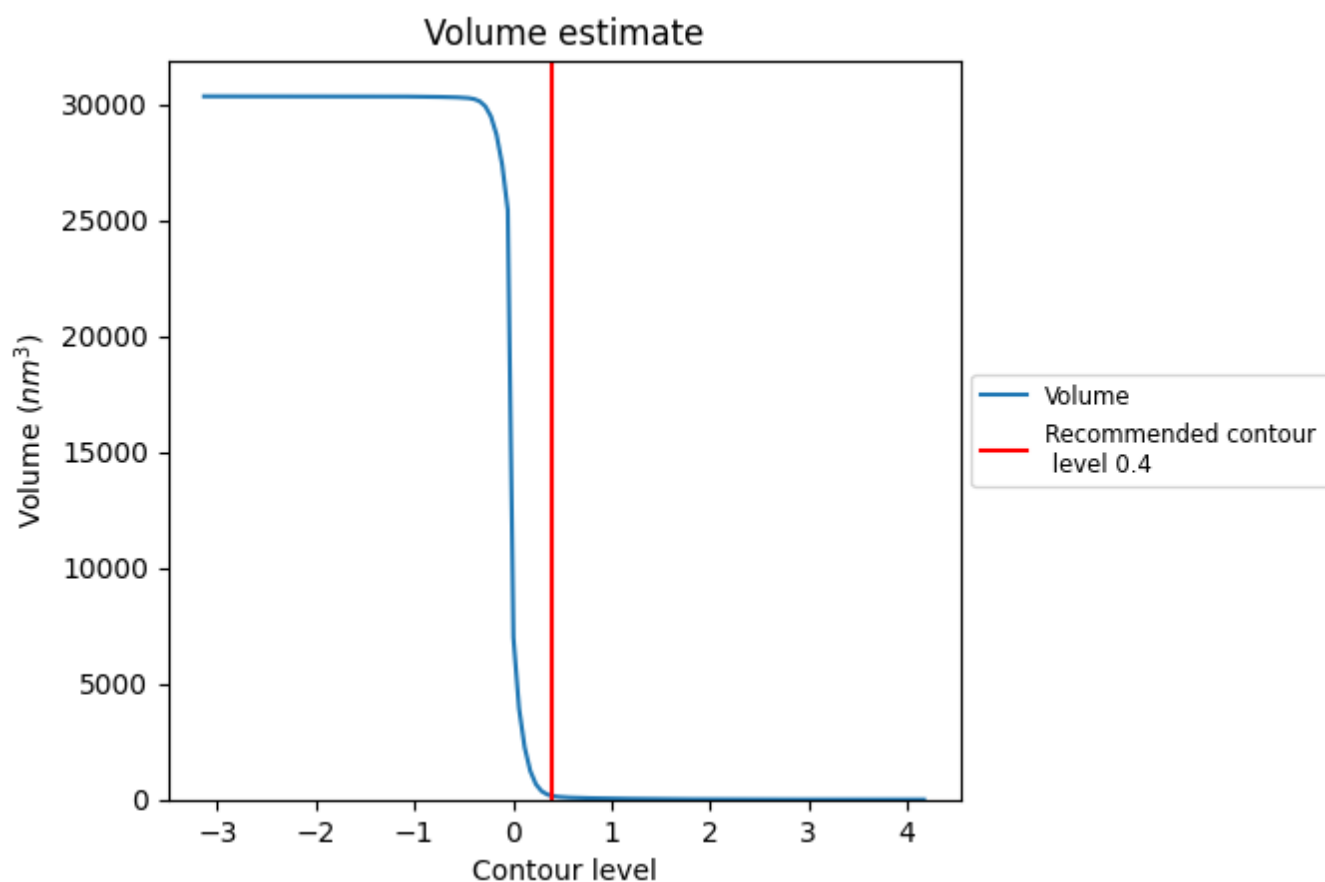
This section contains the results of statistical analysis of the map.

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.

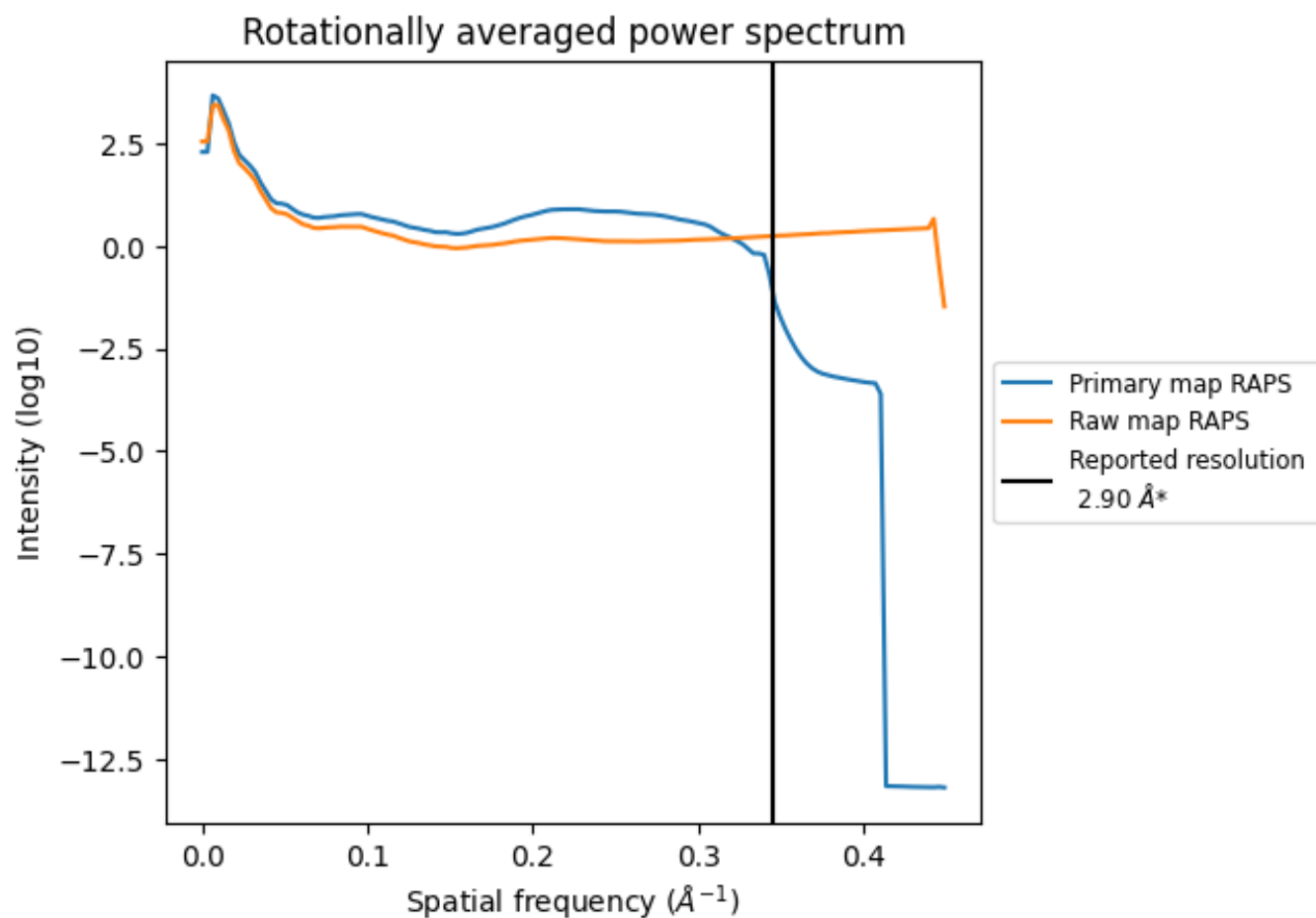
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 ⓘ

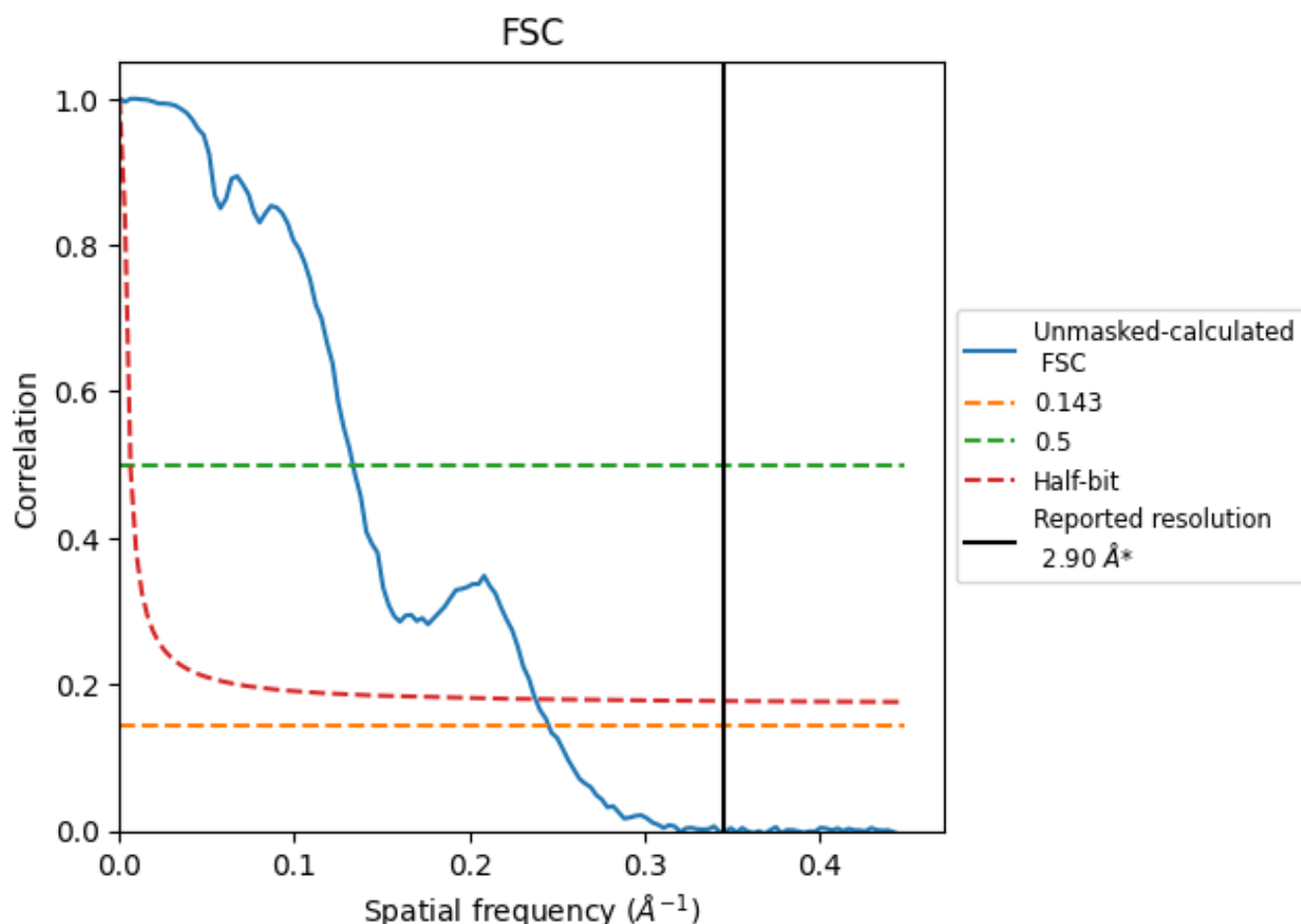


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

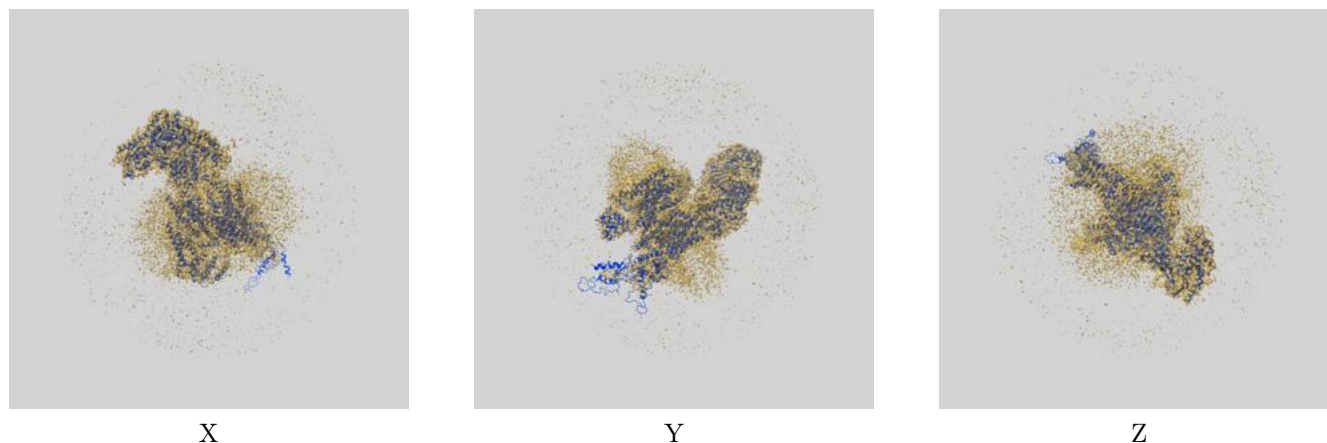
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	7.50	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 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-37472 and PDB model 8WE6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



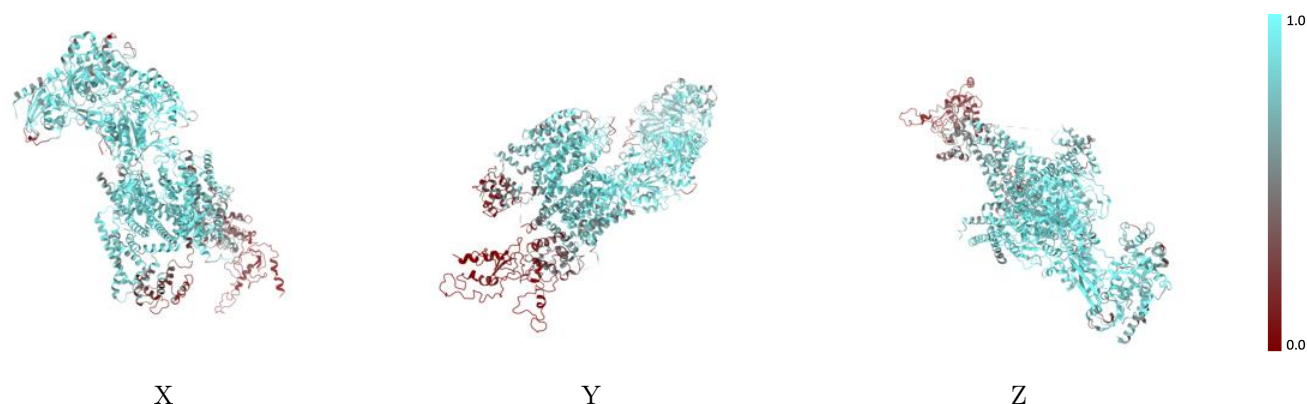
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



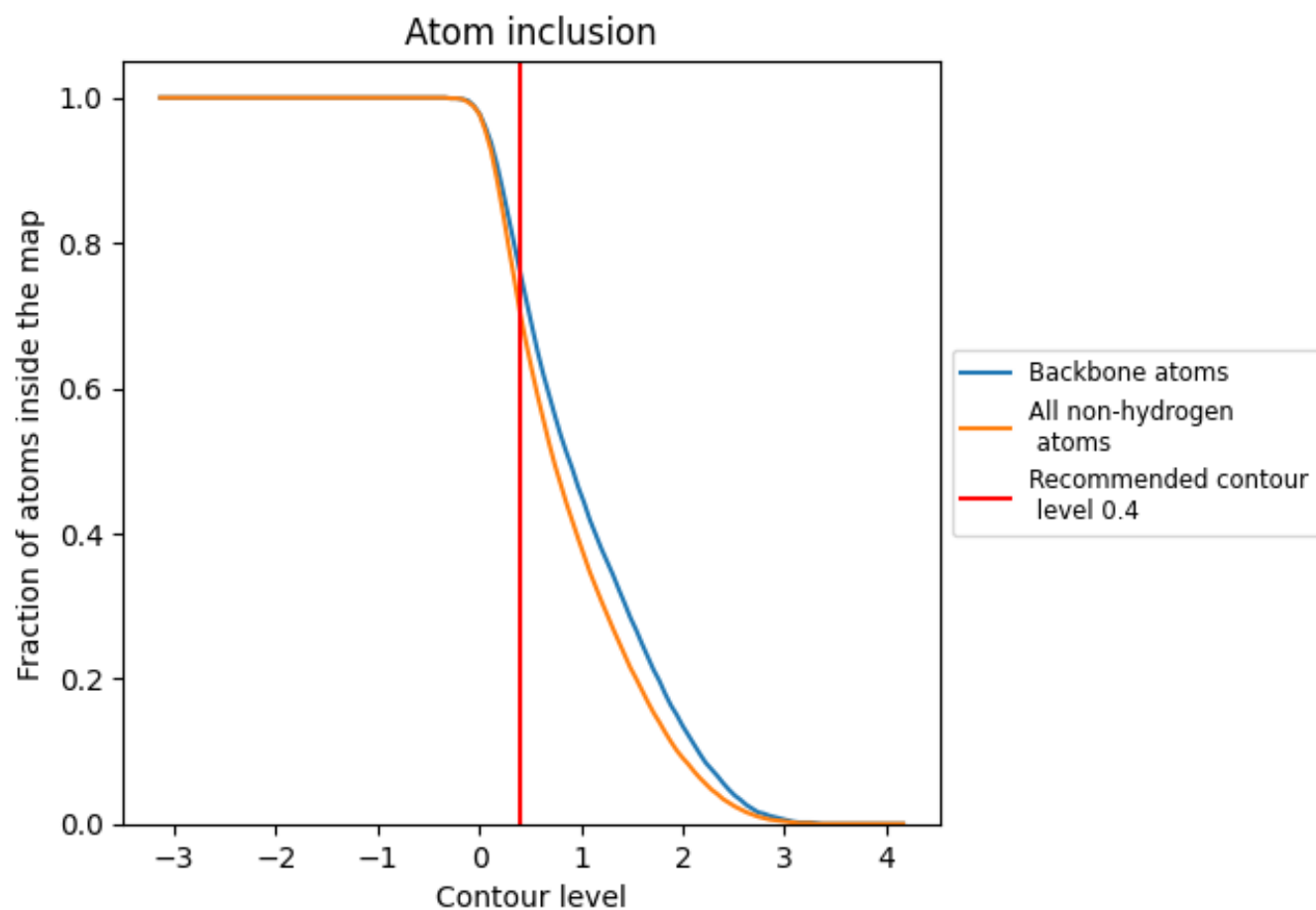
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.4910
A	<div></div> 0.7500	<div></div> 0.5040
B	<div></div> 0.5480	<div></div> 0.3960
C	<div></div> 0.1540	<div></div> 0.3170
D	<div></div> 0.8360	<div></div> 0.5340
E	<div></div> 0.3570	<div></div> 0.2650
F	<div></div> 0.6960	<div></div> 0.4290
G	<div></div> 0.5360	<div></div> 0.4220
H	<div></div> 0.5710	<div></div> 0.3370

