



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:54 PM UTC

PDB ID : 8WE8 / pdb_00008we8
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

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:

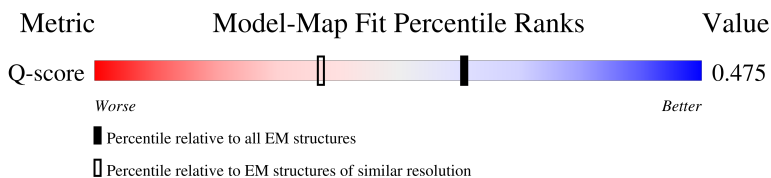
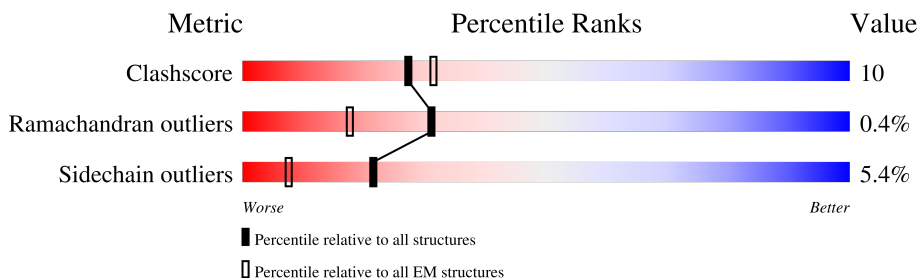
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	60	

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Mol	Chain	Length	Quality of chain
5	E	3	33% 67% 33%
6	F	2	100% 50% 50%
6	H	2	50% 100%
6	I	2	100%
7	G	4	50% 50%

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		

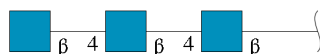
- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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.

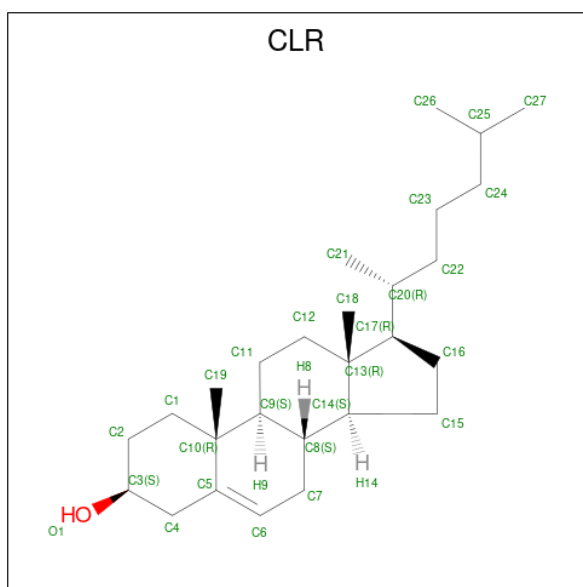


Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 8 is CALCIUM ION (CCD ID: 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 (CCD ID: CLR) (formula: C₂₇H₄₆O).



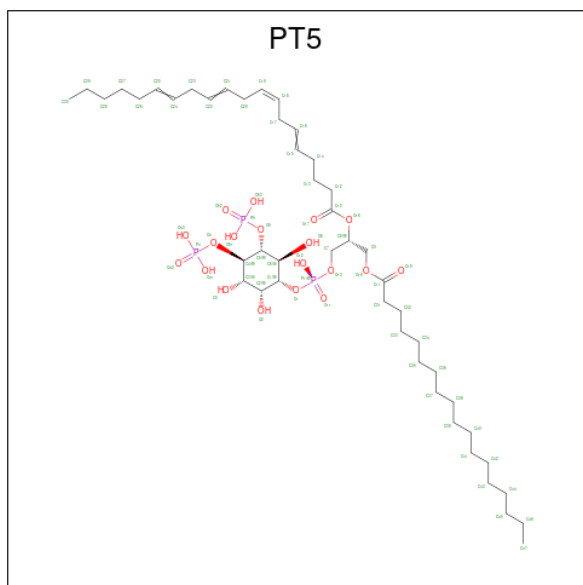
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	B	1	Total	C	O	0
			28	27	1	

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



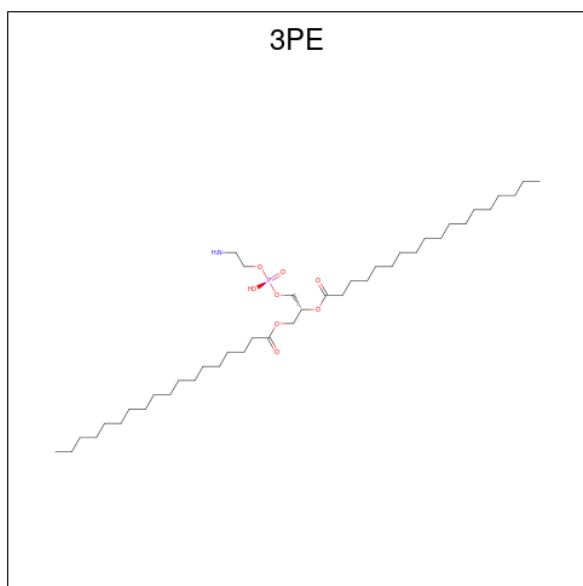
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	

- 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 (CCD ID: PT5) (formula: C₄₇H₈₅O₁₉P₃).



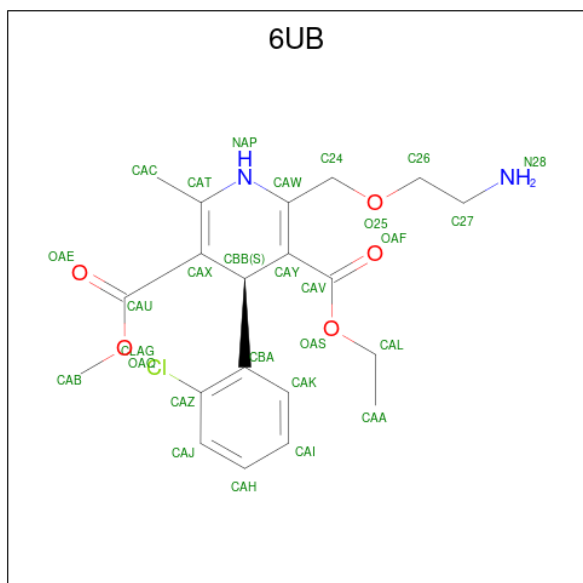
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			63	41	19	3	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 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 (CCD ID: 6UB) (formula: $C_{20}H_{25}ClN_2O_5$).

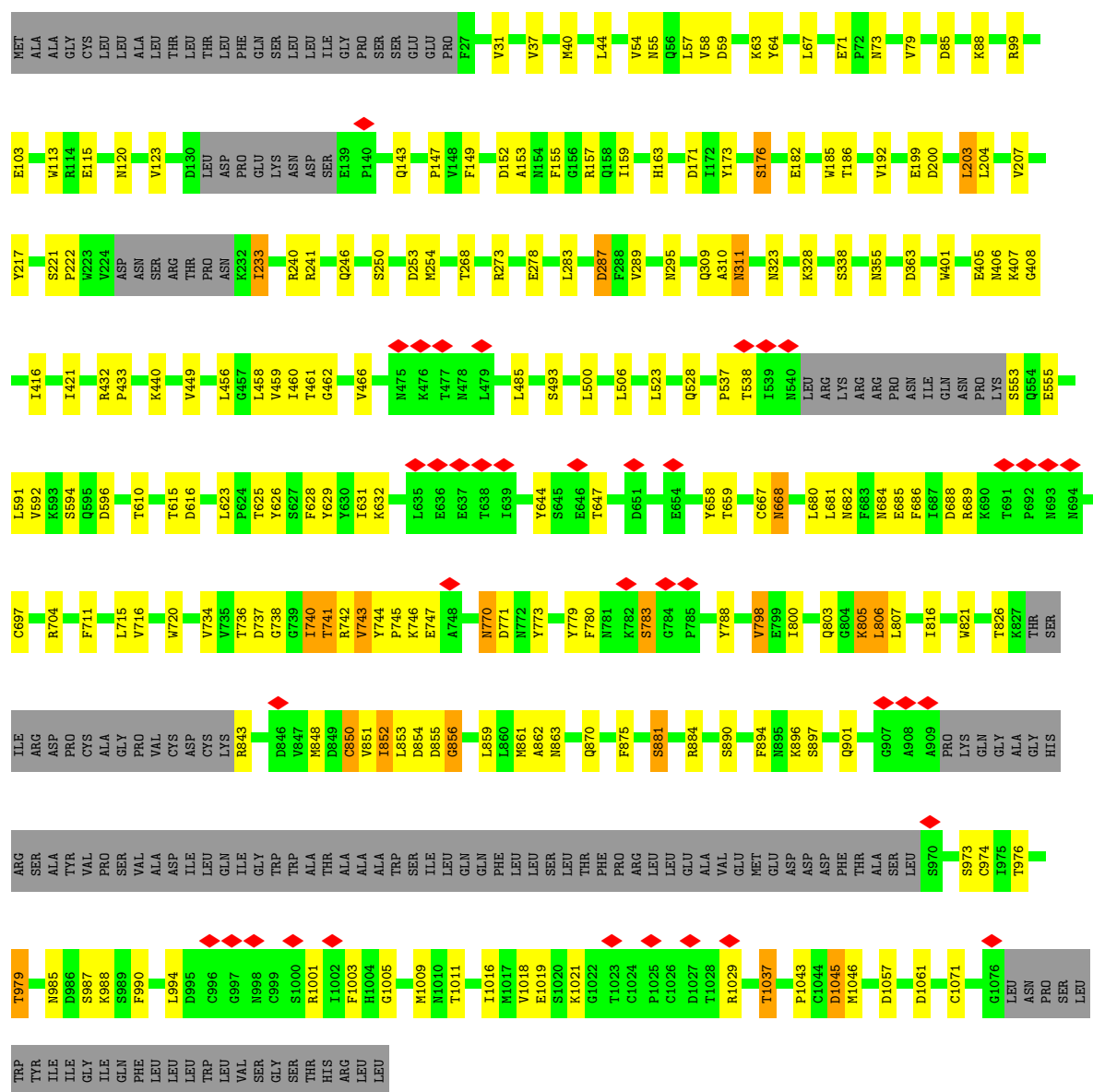


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
13	A	1	28	20	1	2	5	0

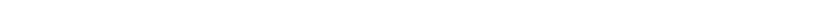


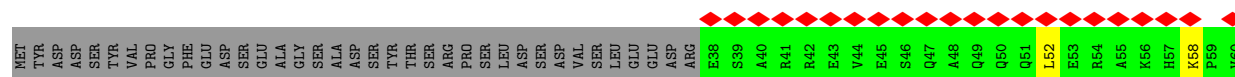
- Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

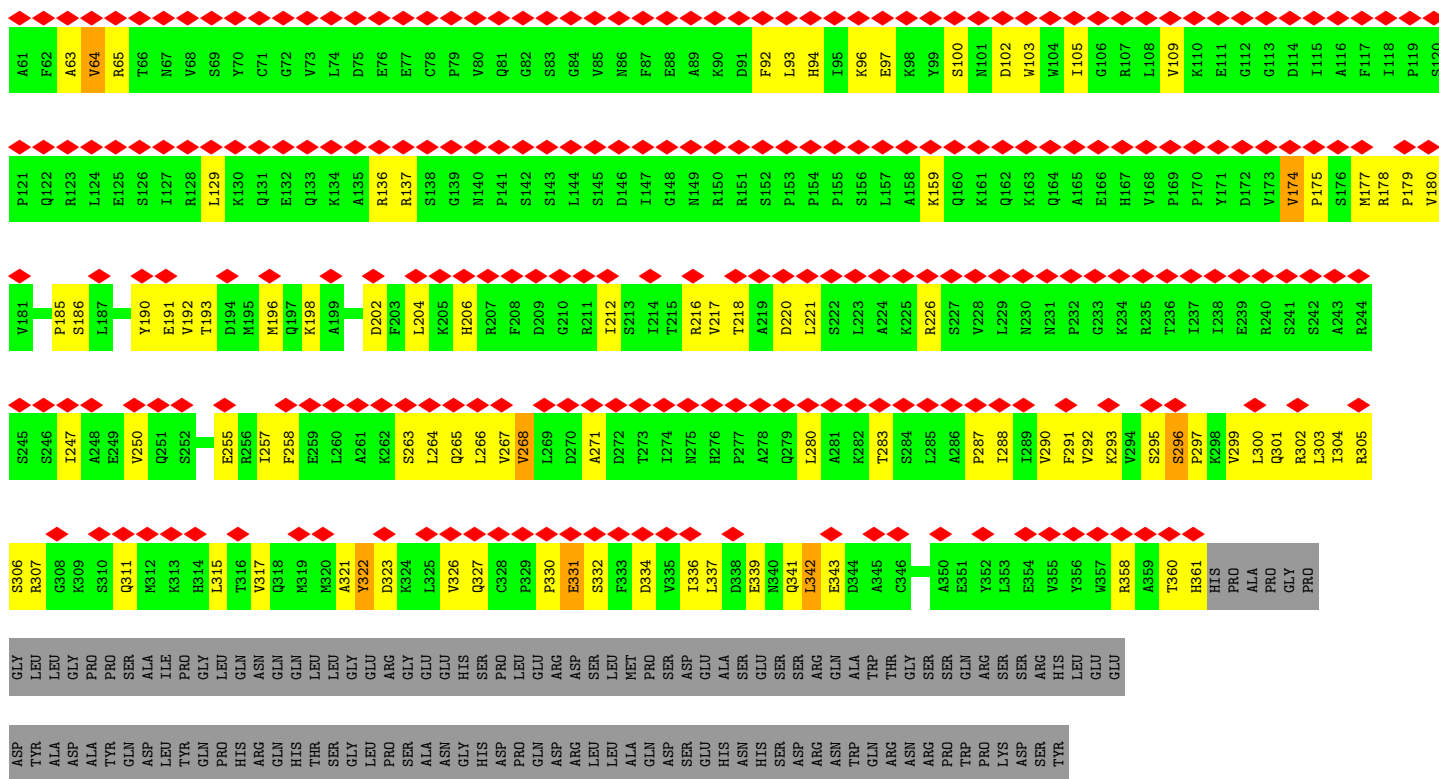
Chain D: 67% 17% 14%



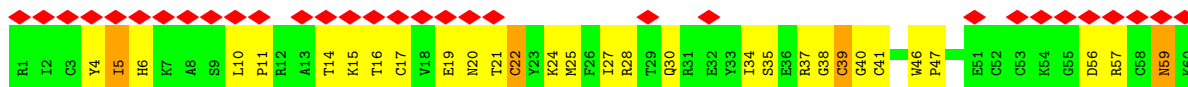
- Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:  56% 47% 18% 33%





- 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-(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: CA, PT5, 3PE, NAG, CLR, 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	1/10414 (0.0%)	0.43	12/14109 (0.1%)
2	D	0.13	0/7728	0.29	0/10477
3	C	0.11	0/2624	0.28	0/3544
4	B	0.17	0/496	0.49	0/664
All	All	0.22	1/21262 (0.0%)	0.37	12/28794 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	909	PHE	CA-C	-5.48	1.45	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1290	LEU	N-CA-C	-12.64	97.51	113.43
1	A	174	ALA	N-CA-C	-10.74	100.67	113.88
1	A	138	CYS	N-CA-C	-9.68	102.56	114.75
1	A	137	ASN	N-CA-C	-8.00	102.83	112.59
1	A	907	LEU	N-CA-C	-7.38	104.27	113.28
1	A	909	PHE	N-CA-C	-6.71	104.04	111.36
1	A	908	PHE	N-CA-C	-5.96	104.17	112.45
1	A	140	ALA	N-CA-C	-5.81	105.08	114.09
1	A	141	LEU	N-CA-C	-5.78	105.55	113.30
1	A	902	PHE	N-CA-C	-5.29	104.56	111.02
1	A	1008	SER	CB-CA-C	-5.22	110.12	117.23
1	A	169	ILE	O-C-N	-5.13	116.57	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10183	0	10404	208	0
2	D	7570	0	7369	128	0
3	C	2575	0	2619	64	0
4	B	486	0	474	22	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	4	0
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	417	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 10.

All (417) 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
3:C:177:MET:HE2	3:C:266:LEU:HG	1.60	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1226:ASN:C	1:A:1228:HIS:H	2.01	0.68
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
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: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:1605:MET:HE1	1:A:1607:ASN:HB2	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: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:1255:CYS:HA	1:A:1258:MET:HE2	1.84	0.60
1:A:583:TYR:HH	1:A:593:CYS:HG	1.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:902:PHE:O	1:A:903:THR:C	2.44	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
1:A:1204:LYS:O	1:A:1204:LYS:HG2	2.01	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:682:MET:HE3	1:A:1099:GLY:HA3	1.84	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
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
2:D:821:TRP:CD2	2:D:861:MET:HE1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:988:LYS:HD3	2:D:1009:MET:HE2	1.87	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
1:A:592:ASP:O	1:A:596:VAL:HG23	2.05	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
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:1225:LYS:C	1:A:1227:GLN:H	2.16	0.54
1:A:1389:SER:O	1:A:1389:SER:OG	2.24	0.54
1:A:1422:TYR:O	1:A:1503:TYR:OH	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
1:A:1226:ASN:C	1:A:1228:HIS:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:615:THR:OG1	2:D:616:ASP:N	2.39	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
1:A:904:ASN:O	1:A:905:LEU:C	2.51	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
2:D:747:GLU:H	2:D:747:GLU:CD	2.16	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:605:LEU:C	1:A:607:GLU:H	2.19	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
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
2:D:113:TRP:CD1	7:G:3:NAG:HN2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HE2	1:A:196:ASN:HB3	1.94	0.49
1:A:1126:MET:HE1	4:B:46:TRP:CD2	2.47	0.49
2:D:821:TRP:CE2	2:D:861:MET:HE1	2.47	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
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:177:MET:HE3	3:C:178:ARG:O	2.13	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
1:A:1291:ILE:O	1:A:1292:ALA:C	2.55	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: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
4:B:22:CYS:HB2	4:B:59:ASN:HD21	1.79	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
1:A:1245:MET:HE2	1:A:1285:GLU:OE2	2.14	0.47
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:1218:PRO:HG3	1:A:1549:TRP:HE1	1.79	0.47
1:A:175:PHE:CD2	1:A:175:PHE:C	2.93	0.47
1:A:895:ARG:HG3	1:A:974:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:PRO:HG3	1:A:1233:TRP:CB	2.44	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
2:D:644:TYR:O	2:D:647:THR:OG1	2.33	0.46
2:D:861:MET:HB2	2:D:861:MET:HE2	1.72	0.46
3:C:303:LEU:O	3:C:306:SER:OG	2.29	0.46
9:B:101:CLR:H162	9:B:101:CLR:H221	1.65	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:1222:TYR:CD1	1:A:1222:TYR:C	2.94	0.46
1:A:1618:LEU:HD12	1:A:1619:ARG:HB2	1.98	0.46
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:1225:LYS:C	1:A:1227:GLN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	2:D:688:ASP:N	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
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
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
2:D:632:LYS:HB3	2:D:632:LYS:HZ2	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:1245:MET:HB3	1:A:1245:MET:HE3	1.78	0.44
6:F:2:NAG:O7	6:F:2:NAG:O4	2.20	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1600:SER:H	1:A:1603:THR:HG1	1.65	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:331:GLU:CD	3:C:332:SER:H	2.26	0.43
1:A:583:TYR:OH	1:A:593:CYS:SG	2.63	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
3:C:255:GLU:H	3:C:255:GLU:CD	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:282:TYR:O	1:A:384:TYR:OH	2.37	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:254:MET:HE3	2:D:283:LEU:HD21	2.01	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:605:LEU:C	1:A:607:GLU:N	2.78	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:OD1	2:D:770:ASN:N	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1126:MET:HE3	1:A:1126:MET:HB3	1.85	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:881:SER:HG	2:D:1021:LYS:HZ2	1.68	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: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:40:MET:HE2	2:D:40:MET:HB2	1.84	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
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
3:C:92:PHE:CZ	3:C:178:ARG:HD2	2.57	0.40
4:B:19:GLU:HG3	4:B:20:ASN:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	21	51
2	D	936/1103 (85%)	885 (95%)	49 (5%)	2 (0%)	43	72
3	C	322/484 (66%)	302 (94%)	19 (6%)	1 (0%)	36	65
4	B	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
All	All	2561/3848 (67%)	2397 (94%)	153 (6%)	11 (0%)	31	59

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%)	1054 (94%)	64 (6%)	18	49
2	D	837/971 (86%)	795 (95%)	42 (5%)	22	53
3	C	287/426 (67%)	274 (96%)	13 (4%)	24	58
4	B	54/54 (100%)	48 (89%)	6 (11%)	6	20
All	All	2296/3347 (69%)	2171 (95%)	125 (5%)	21	51

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	163	GLU
1	A	172	VAL
1	A	175	PHE
1	A	178	VAL
1	A	191	LEU
1	A	217	LYS
1	A	253	SER
1	A	257	VAL
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	536	LEU
1	A	570	GLU
1	A	585	VAL
1	A	593	CYS
1	A	597	CYS
1	A	614	LEU
1	A	617	SER
1	A	636	SER
1	A	637	LEU
1	A	638	SER
1	A	657	LEU
1	A	691	ASN
1	A	711	VAL
1	A	761	SER
1	A	898	ASN
1	A	900	THR
1	A	905	LEU
1	A	907	LEU

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Mol	Chain	Res	Type
1	A	908	PHE
1	A	923	VAL
1	A	962	SER
1	A	986	ARG
1	A	992	LEU
1	A	1001	LEU
1	A	1011	ILE
1	A	1042	VAL
1	A	1077	THR
1	A	1095	THR
1	A	1101	VAL
1	A	1141	LEU
1	A	1180	ILE
1	A	1200	CYS
1	A	1221	ARG
1	A	1225	LYS
1	A	1275	ASN
1	A	1281	LEU
1	A	1288	LEU
1	A	1289	LYS
1	A	1290	LEU
1	A	1305	VAL
1	A	1309	LEU
1	A	1381	VAL
1	A	1389	SER
1	A	1392	GLU
1	A	1394	ILE
1	A	1418	LEU
1	A	1467	GLN
1	A	1483	SER
1	A	1515	ILE
2	D	31	VAL
2	D	37	VAL
2	D	176	SER
2	D	203	LEU
2	D	233	ILE
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	421	ILE
2	D	460	ILE
2	D	506	LEU
2	D	523	LEU
2	D	538	THR
2	D	553	SER
2	D	555	GLU
2	D	591	LEU
2	D	592	VAL
2	D	668	ASN
2	D	682	ASN
2	D	734	VAL
2	D	740	ILE
2	D	741	THR
2	D	743	VAL
2	D	770	ASN
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	850	CYS
2	D	852	ILE
2	D	881	SER
2	D	897	SER
2	D	973	SER
2	D	979	THR
2	D	1037	THR
2	D	1045	ASP
2	D	1071	CYS
3	C	64	VAL
3	C	109	VAL
3	C	174	VAL
3	C	186	SER
3	C	192	VAL
3	C	257	ILE
3	C	267	VAL
3	C	268	VAL
3	C	290	VAL
3	C	296	SER
3	C	315	LEU

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Mol	Chain	Res	Type
3	C	322	TYR
3	C	342	LEU
4	B	5	ILE
4	B	14	THR
4	B	22	CYS
4	B	39	CYS
4	B	41	CYS
4	B	59	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS
1	A	348	ASN
1	A	358	GLN
1	A	429	GLN
1	A	548	GLN
1	A	550	ASN
1	A	556	GLN
1	A	694	GLN
1	A	741	ASN
1	A	746	ASN
1	A	898	ASN
1	A	904	ASN
1	A	1092	ASN
1	A	1445	ASN
1	A	1517	ASN
1	A	1573	GLN
2	D	111	HIS
2	D	314	ASN
2	D	370	GLN
2	D	391	GLN
2	D	641	GLN
2	D	684	ASN
2	D	863	ASN
2	D	864	HIS
2	D	901	GLN
3	C	50	GLN
3	C	149	ASN

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	0.61	0	17,19,21	2.05	3 (17%)
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	E	3	5	14,14,15	0.34	0	17,19,21	0.40	0
6	NAG	F	1	6,2	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
6	NAG	F	2	6	14,14,15	0.63	1 (7%)	17,19,21	0.82	0
7	NAG	G	1	2,7	14,14,15	0.26	0	17,19,21	0.49	0
7	NAG	G	2	7	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	G	3	7	14,14,15	1.01	1 (7%)	17,19,21	1.72	2 (11%)
7	NAG	G	4	7	14,14,15	0.54	0	17,19,21	1.33	2 (11%)
6	NAG	H	1	6,2	14,14,15	0.28	0	17,19,21	0.45	0
6	NAG	H	2	6	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	I	1	6,2	14,14,15	0.53	0	17,19,21	0.42	0
6	NAG	I	2	6	14,14,15	0.23	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
7	NAG	G	1	2,7	-	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	-	6/6/23/26	0/1/1/1
7	NAG	G	4	7	-	6/6/23/26	0/1/1/1
6	NAG	H	1	6,2	-	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	6,2	-	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	3.17	1.49	1.43
6	F	2	NAG	O5-C1	-2.17	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	7.34	122.02	112.19
7	G	3	NAG	C1-O5-C5	4.63	118.40	112.19
7	G	3	NAG	C2-N2-C7	4.63	129.10	122.90
7	G	4	NAG	C2-N2-C7	4.56	129.01	122.90
5	E	1	NAG	C3-C4-C5	2.99	115.65	110.23
5	E	1	NAG	O5-C5-C4	2.56	117.06	110.83
6	F	1	NAG	C1-O5-C5	2.56	115.61	112.19
7	G	4	NAG	C1-C2-N2	2.17	113.85	110.43

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	3	NAG	O5-C5-C6-O6
7	G	3	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
7	G	4	NAG	C4-C5-C6-O6

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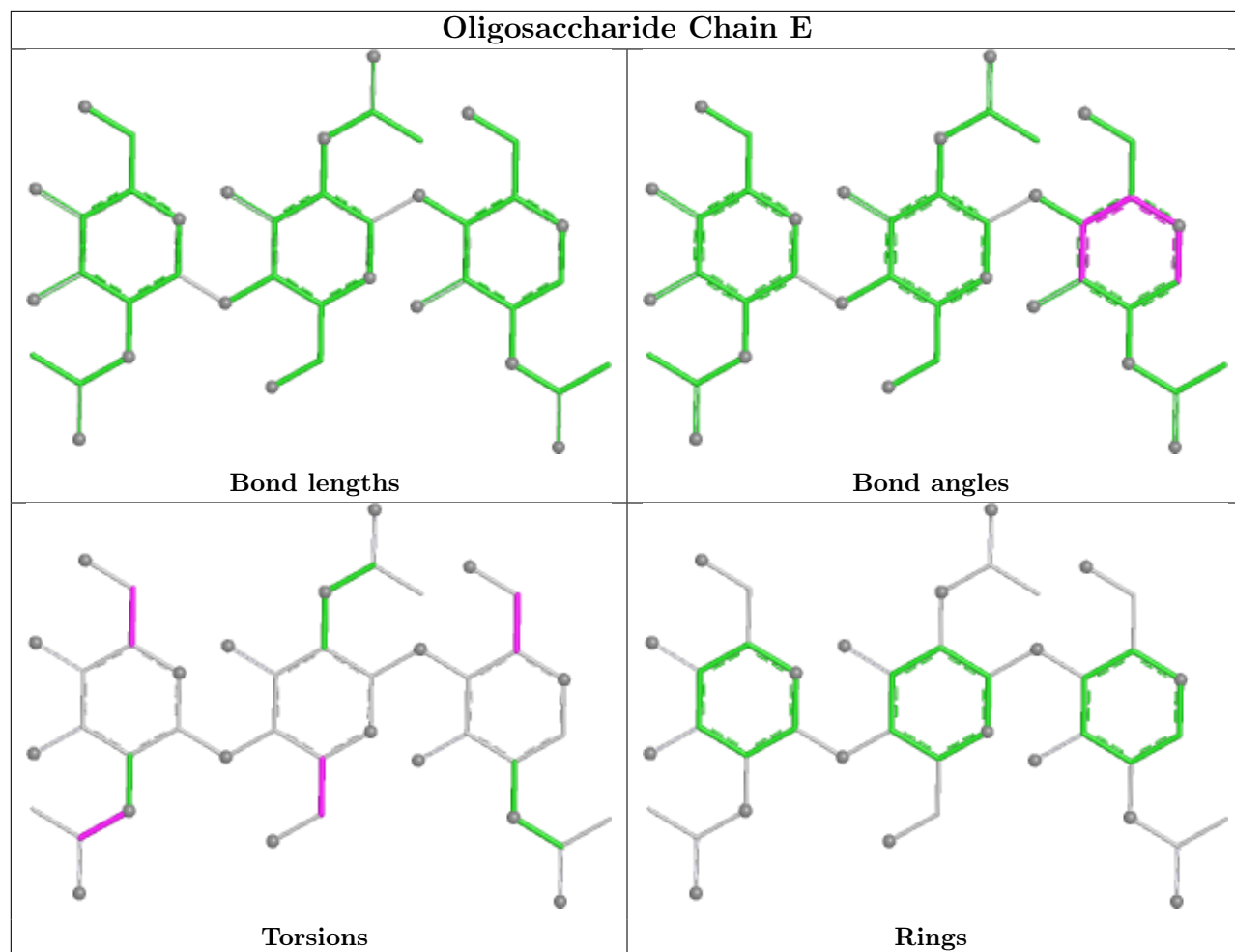
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
7	G	4	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
5	E	3	NAG	C8-C7-N2-C2
5	E	3	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
7	G	3	NAG	C8-C7-N2-C2
7	G	3	NAG	O7-C7-N2-C2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

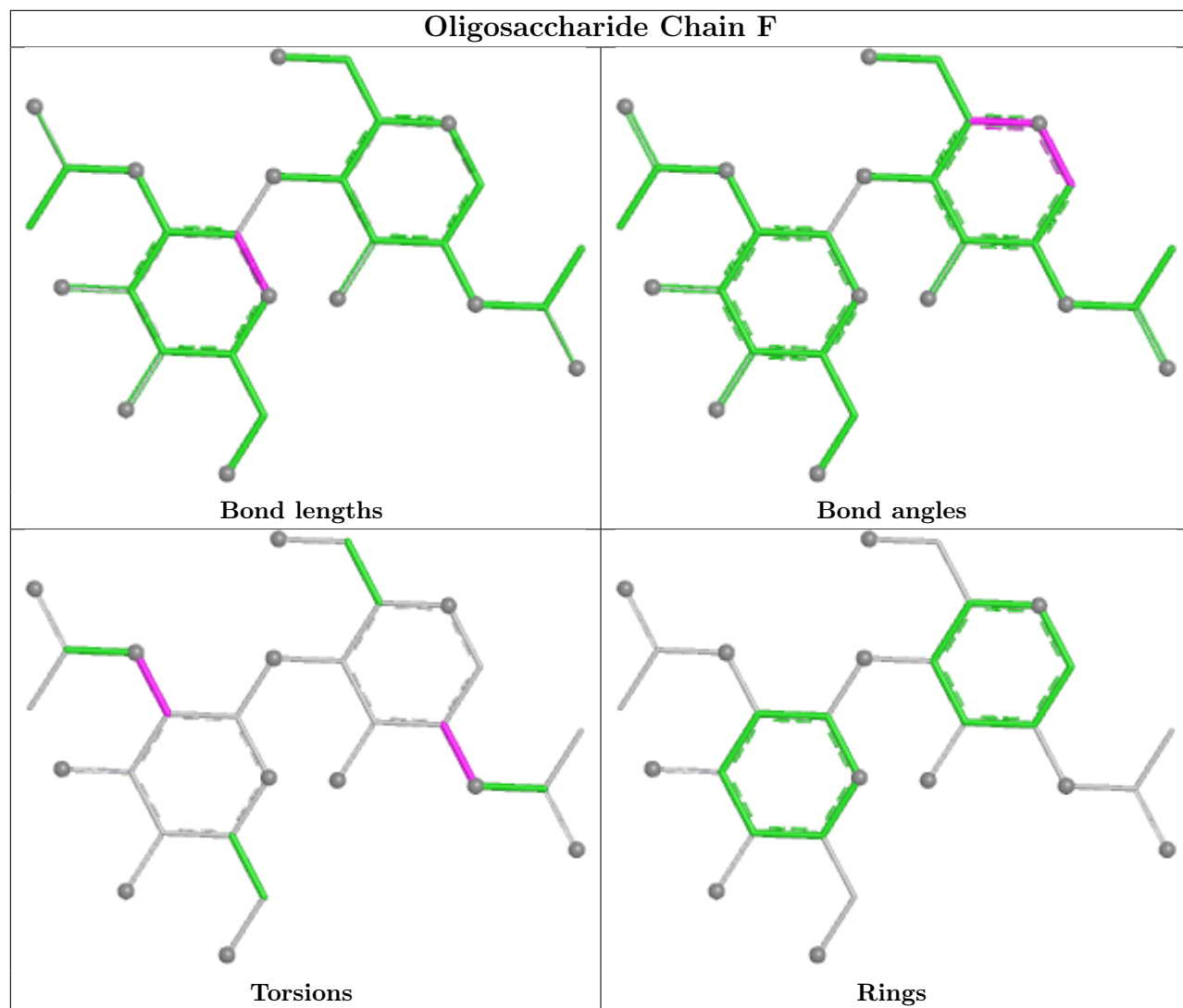
There are no ring outliers.

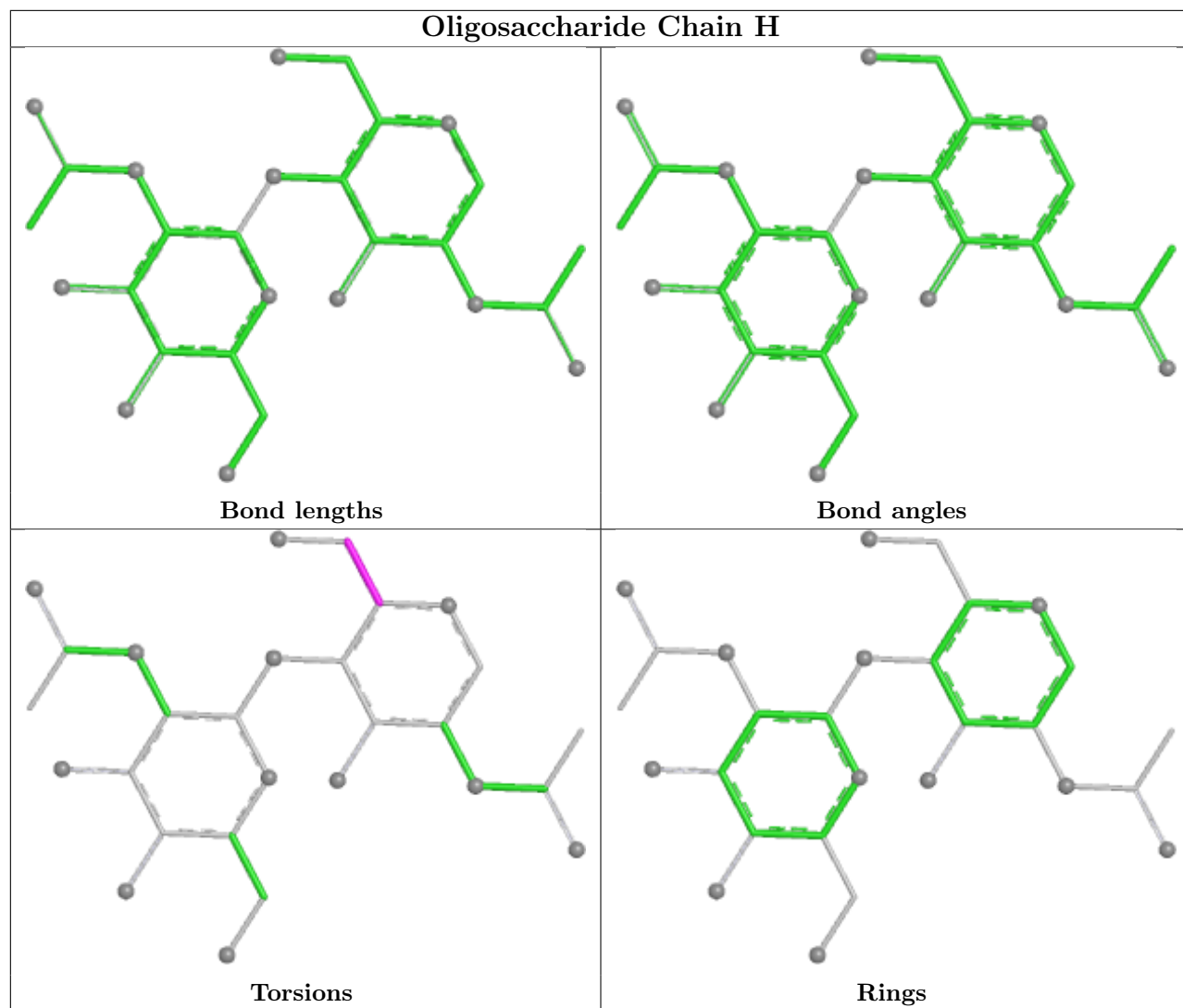
4 monomers are involved in 7 short contacts:

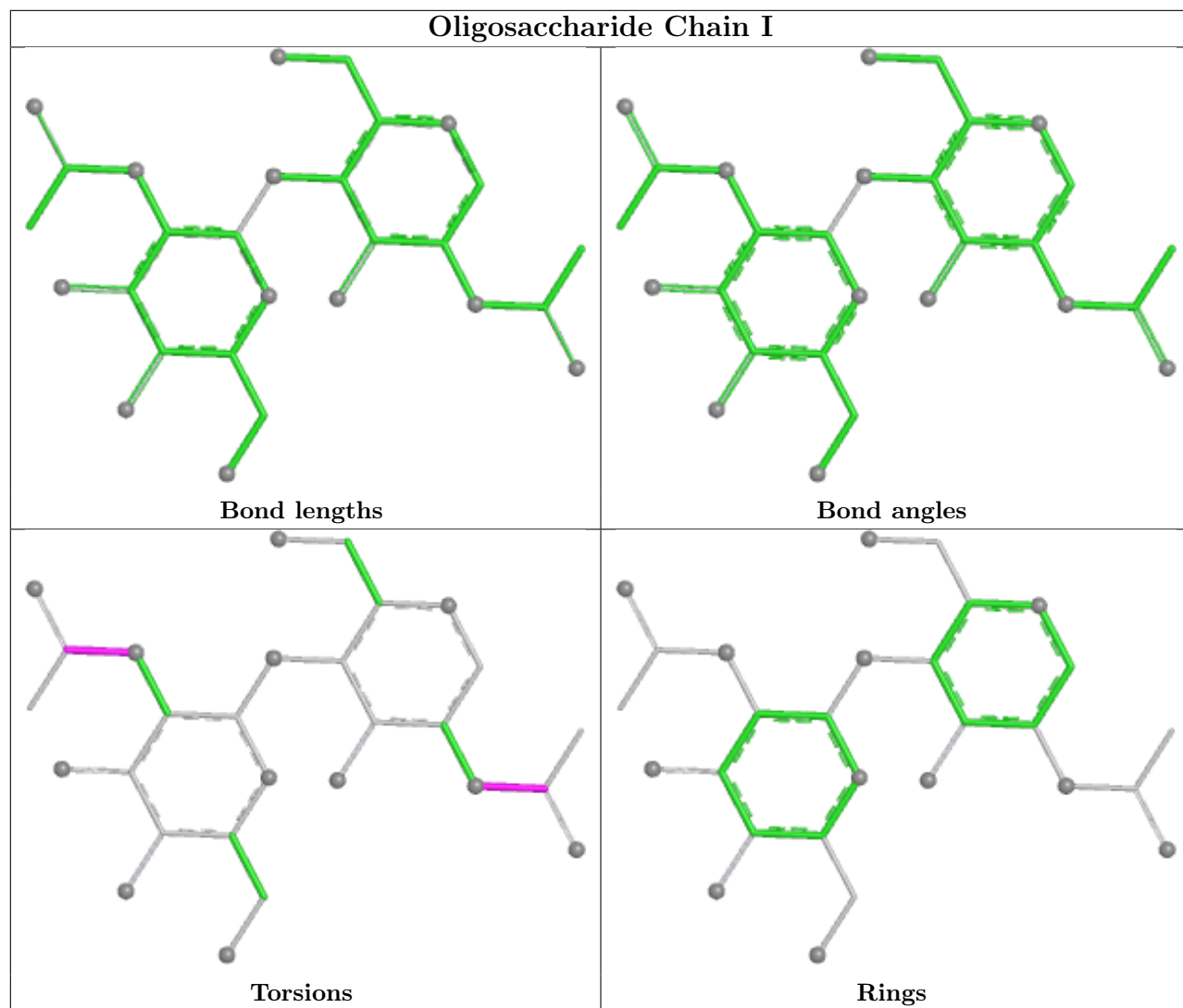
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
7	G	3	NAG	3	0
7	G	4	NAG	1	0
6	F	2	NAG	1	0

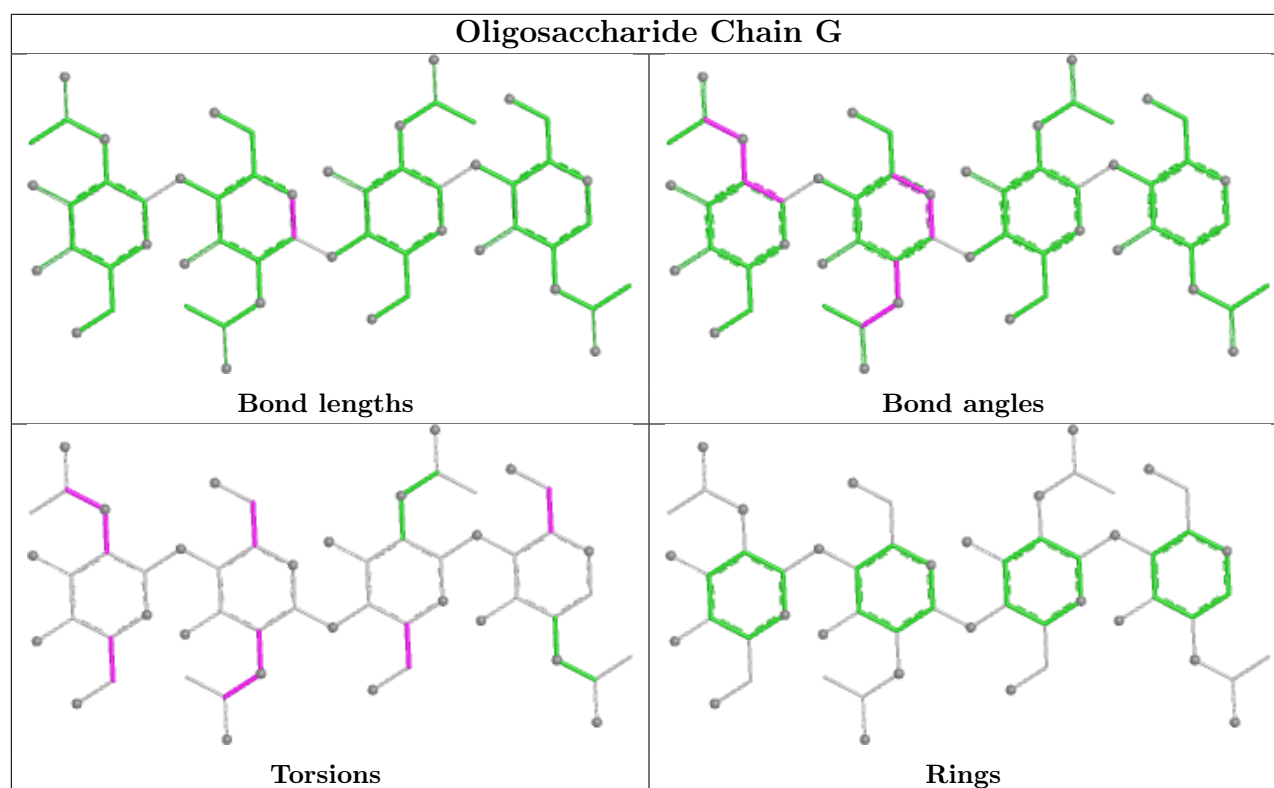
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 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
12	3PE	A	2308	-	37,37,50	0.58	0	40,42,55	0.61	1 (2%)
9	CLR	A	2302	-	31,31,31	0.37	0	48,48,48	0.57	0
10	NAG	D	1203	2	14,14,15	0.85	1 (7%)	17,19,21	1.04	1 (5%)
9	CLR	A	2304	-	31,31,31	0.40	0	48,48,48	0.80	1 (2%)
10	NAG	A	2306	1	14,14,15	0.31	0	17,19,21	0.43	0
13	6UB	A	2309	-	28,29,29	2.08	12 (42%)	38,39,39	2.46	14 (36%)
10	NAG	D	1202	2	14,14,15	0.36	0	17,19,21	0.53	0
9	CLR	A	2303	-	31,31,31	0.38	0	48,48,48	0.53	0
9	CLR	A	2305	-	31,31,31	0.40	0	48,48,48	0.77	1 (2%)
9	CLR	B	101	-	31,31,31	0.37	0	48,48,48	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PT5	A	2307	-	63,63,69	0.87	2 (3%)	78,81,87	1.04	3 (3%)

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	2309	6UB	CAT-CAX	-4.20	1.30	1.35
11	A	2307	PT5	O18-C11	4.05	1.45	1.33
13	A	2309	6UB	CAW-NAP	3.99	1.43	1.37
11	A	2307	PT5	O16-C10	3.98	1.45	1.34
13	A	2309	6UB	CAT-NAP	3.43	1.43	1.38
13	A	2309	6UB	CAV-CAY	3.26	1.53	1.47
13	A	2309	6UB	OAS-CAV	3.10	1.39	1.33
10	D	1203	NAG	O5-C1	2.75	1.48	1.43
13	A	2309	6UB	OAQ-CAB	-2.64	1.39	1.45
13	A	2309	6UB	CAU-CAX	2.61	1.52	1.47
13	A	2309	6UB	OAQ-CAU	2.33	1.38	1.33
13	A	2309	6UB	CAW-CAY	-2.17	1.33	1.36
13	A	2309	6UB	CBB-CAY	2.13	1.54	1.52
13	A	2309	6UB	OAS-CAL	-2.08	1.40	1.46
13	A	2309	6UB	OAF-CAV	-2.05	1.17	1.21

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	2309	6UB	CAC-CAT-CAX	-7.35	120.30	127.61
13	A	2309	6UB	CBA-CAZ-CLAG	5.92	126.47	120.41
13	A	2309	6UB	OAS-CAV-CAY	4.72	120.78	112.28
10	D	1203	NAG	C1-O5-C5	4.06	117.63	112.19
11	A	2307	PT5	O16-C10-C12	3.96	120.05	111.48
13	A	2309	6UB	OAQ-CAU-CAX	3.64	119.01	112.31
13	A	2309	6UB	CAK-CBA-CBB	-3.40	113.11	119.39
13	A	2309	6UB	CAL-OAS-CAV	-3.36	110.69	116.49
13	A	2309	6UB	CAZ-CBA-CBB	3.31	128.37	123.97
13	A	2309	6UB	CAC-CAT-NAP	3.25	117.19	113.42
11	A	2307	PT5	O18-C11-C31	3.24	121.71	111.83
13	A	2309	6UB	OAS-CAV-OAF	-3.22	117.59	123.37
13	A	2309	6UB	CAX-CBB-CAY	2.62	114.23	109.78
13	A	2309	6UB	CAJ-CAZ-CBA	-2.51	119.61	121.98
11	A	2307	PT5	O18-C11-O19	-2.51	117.35	123.63
13	A	2309	6UB	OAQ-CAU-OAE	-2.47	118.78	123.50
12	A	2308	3PE	O12-P-O14	2.45	123.84	112.44
13	A	2309	6UB	CAJ-CAZ-CLAG	-2.28	113.92	118.42
13	A	2309	6UB	CBB-CAY-CAV	-2.10	111.94	117.09
9	A	2305	CLR	C17-C13-C14	2.05	102.45	100.10
9	A	2304	CLR	C7-C8-C9	2.01	112.04	109.72

There are no chirality outliers.

All (92) 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	C16-C17-C18-C19
12	A	2308	3PE	C1-O11-P-O12
12	A	2308	3PE	C1-O11-P-O13
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	CAY-CAV-OAS-CAL
13	A	2309	6UB	OAF-CAV-OAS-CAL
9	B	101	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
10	A	2306	NAG	O5-C5-C6-O6
10	D	1203	NAG	C4-C5-C6-O6
9	A	2304	CLR	C21-C20-C22-C23
12	A	2308	3PE	O22-C21-O21-C2
13	A	2309	6UB	CAX-CAU-OAQ-CAB
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	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
9	B	101	CLR	C16-C17-C20-C22
9	A	2304	CLR	C17-C20-C22-C23
9	B	101	CLR	C17-C20-C22-C23
13	A	2309	6UB	OAE-CAU-OAQ-CAB
12	A	2308	3PE	O32-C31-O31-C3
11	A	2307	PT5	C12-C10-O16-C8
11	A	2307	PT5	O17-C10-O16-C8
13	A	2309	6UB	OAE-CAU-CAX-CBB
12	A	2308	3PE	C39-C3A-C3B-C3C
12	A	2308	3PE	C24-C25-C26-C27
11	A	2307	PT5	C33-C34-C35-C36
12	A	2308	3PE	C37-C38-C39-C3A
13	A	2309	6UB	OAQ-CAU-CAX-CBB
9	A	2303	CLR	C20-C22-C23-C24
12	A	2308	3PE	C34-C35-C36-C37
12	A	2308	3PE	C25-C26-C27-C28
11	A	2307	PT5	C31-C11-O18-C9
9	A	2305	CLR	C21-C20-C22-C23
11	A	2307	PT5	C42-C43-C44-C45
11	A	2307	PT5	C7-C8-C9-O18
12	A	2308	3PE	C1-C2-C3-O31
11	A	2307	PT5	C12-C13-C14-C15
9	A	2305	CLR	C22-C23-C24-C25
11	A	2307	PT5	O19-C11-O18-C9
9	A	2304	CLR	C20-C22-C23-C24
12	A	2308	3PE	C26-C27-C28-C29
11	A	2307	PT5	C35-C36-C37-C38
11	A	2307	PT5	C32-C33-C34-C35
13	A	2309	6UB	CAZ-CBA-CBB-CAY
13	A	2309	6UB	CAZ-CBA-CBB-CAX

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Mol	Chain	Res	Type	Atoms
12	A	2308	3PE	O11-C1-C2-O21
13	A	2309	6UB	CAW-C24-O25-C26
12	A	2308	3PE	O21-C2-C3-O31
10	D	1202	NAG	C3-C2-N2-C7
11	A	2307	PT5	C7-O13-P1-O1
12	A	2308	3PE	C1-O11-P-O14
11	A	2307	PT5	C7-C8-O16-C10
13	A	2309	6UB	C27-C26-O25-C24
11	A	2307	PT5	C10-C12-C13-C14
9	A	2303	CLR	C22-C23-C24-C25
11	A	2307	PT5	C5-C4-O4-P4
11	A	2307	PT5	C18-C19-C20-C21
11	A	2307	PT5	C19-C20-C21-C22
11	A	2307	PT5	C5-O5-P5-O52
13	A	2309	6UB	OAE-CAU-CAX-CAT
9	A	2305	CLR	C23-C24-C25-C26
10	D	1202	NAG	C1-C2-N2-C7
12	A	2308	3PE	C36-C37-C38-C39
12	A	2308	3PE	C3B-C3C-C3D-C3E
13	A	2309	6UB	OAQ-CAU-CAX-CAT
9	A	2305	CLR	C23-C24-C25-C27
11	A	2307	PT5	O16-C10-C12-C13
13	A	2309	6UB	CAK-CBA-CBB-CAX
9	A	2303	CLR	C13-C17-C20-C21
9	A	2302	CLR	C13-C17-C20-C21
9	A	2304	CLR	C22-C23-C24-C25
11	A	2307	PT5	C34-C35-C36-C37
11	A	2307	PT5	C41-C42-C43-C44
9	A	2303	CLR	C16-C17-C20-C22
9	A	2303	CLR	C17-C20-C22-C23
9	A	2302	CLR	C16-C17-C20-C22
11	A	2307	PT5	O17-C10-C12-C13
12	A	2308	3PE	O11-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

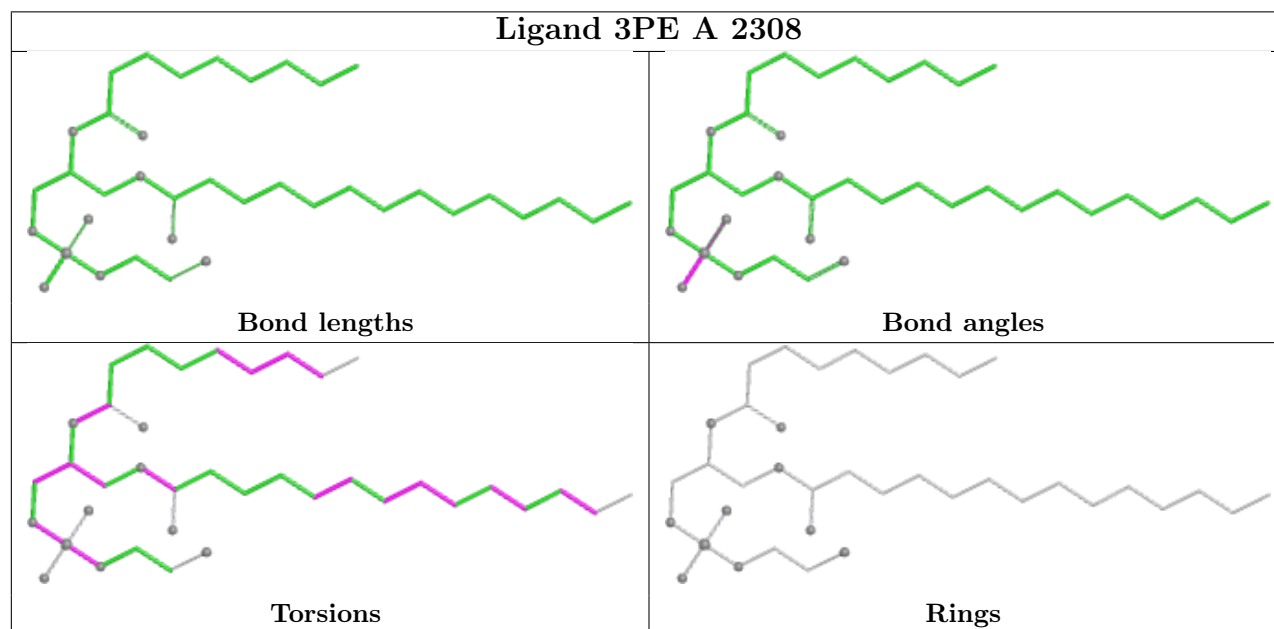
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2302	CLR	1	0
9	A	2304	CLR	3	0
10	D	1202	NAG	1	0
9	A	2303	CLR	2	0

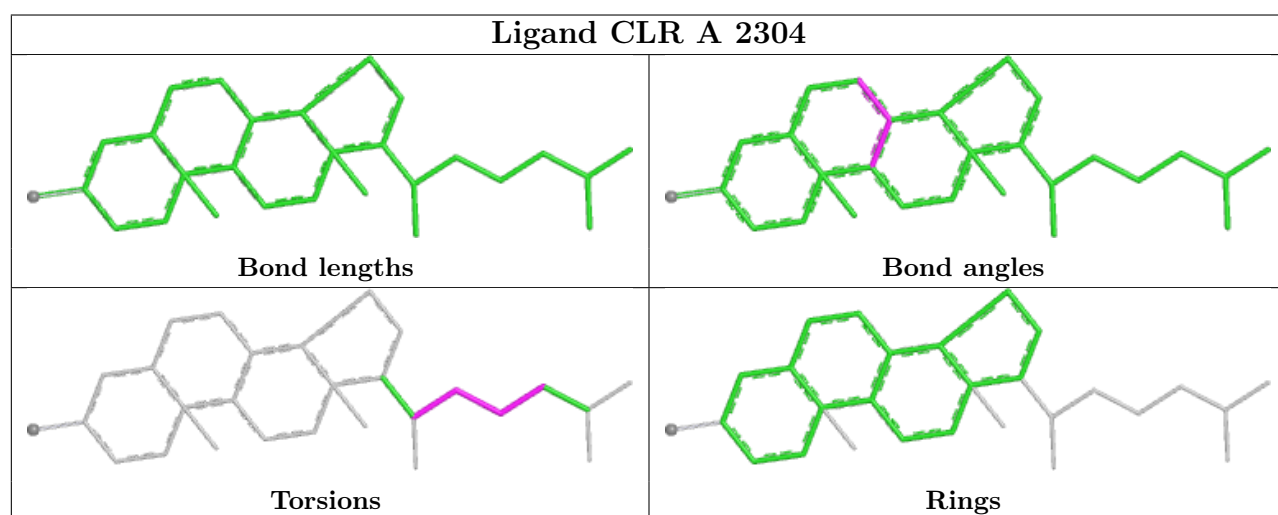
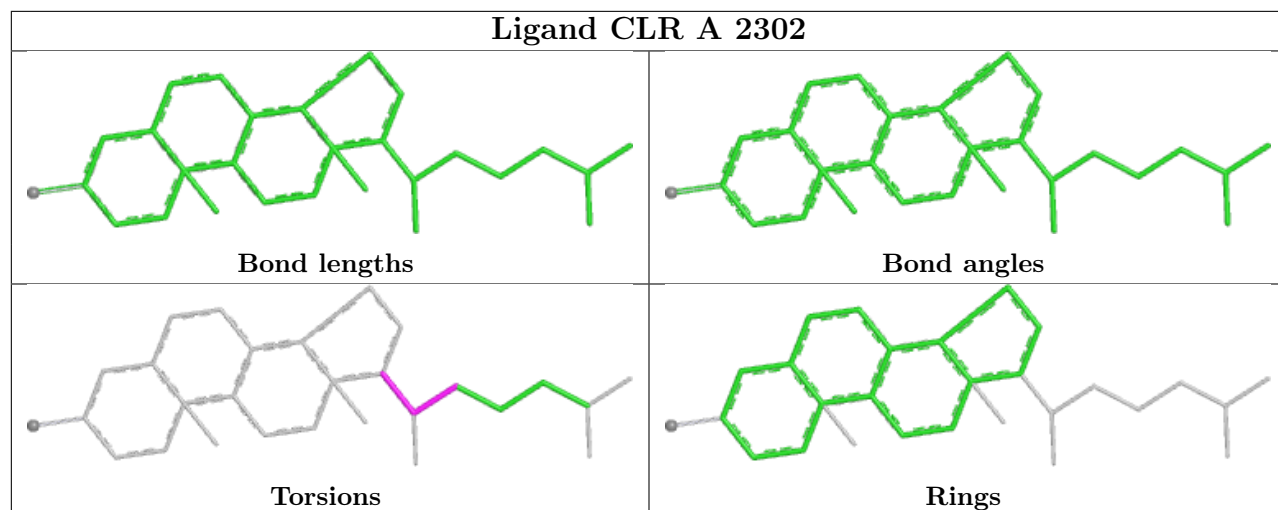
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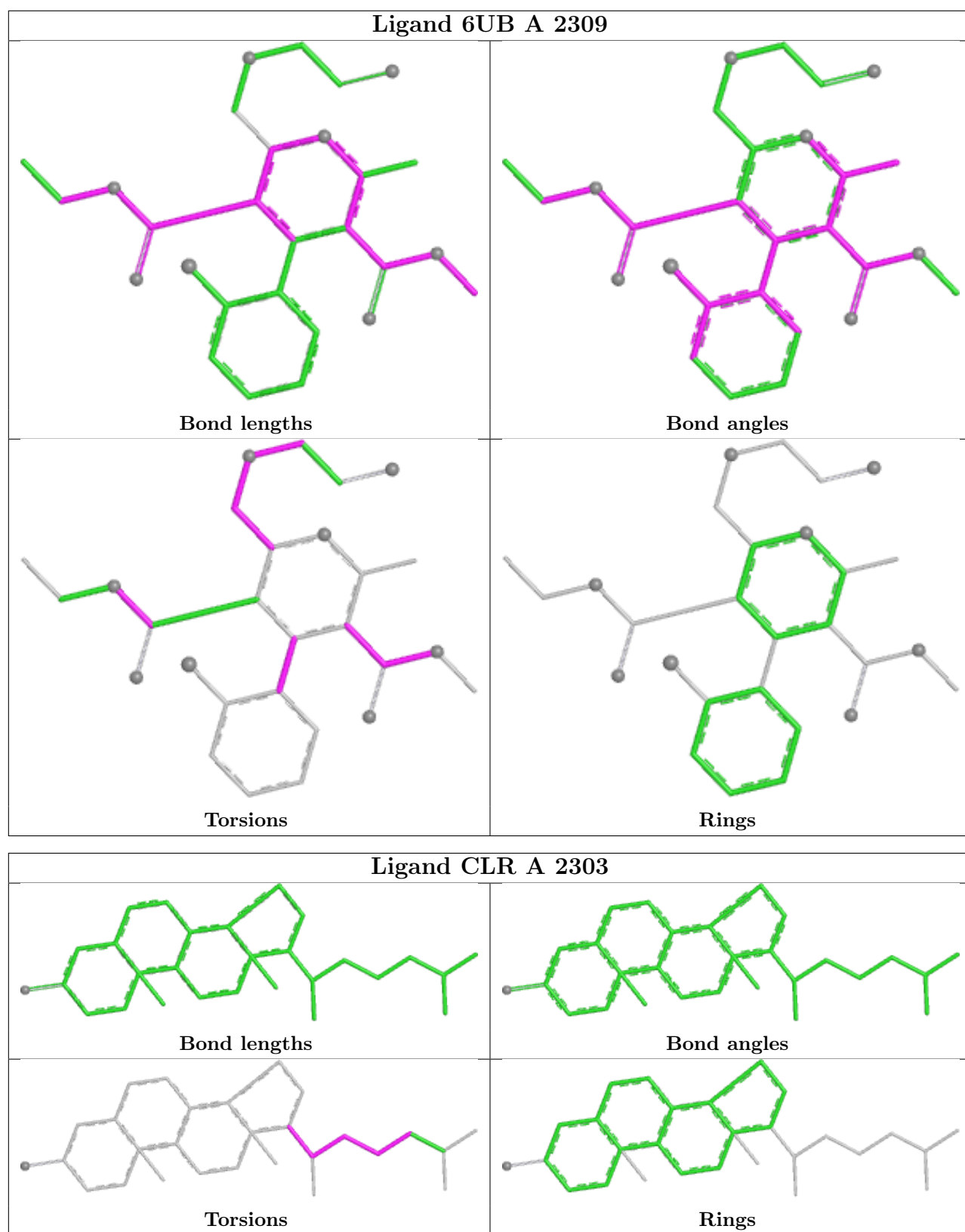
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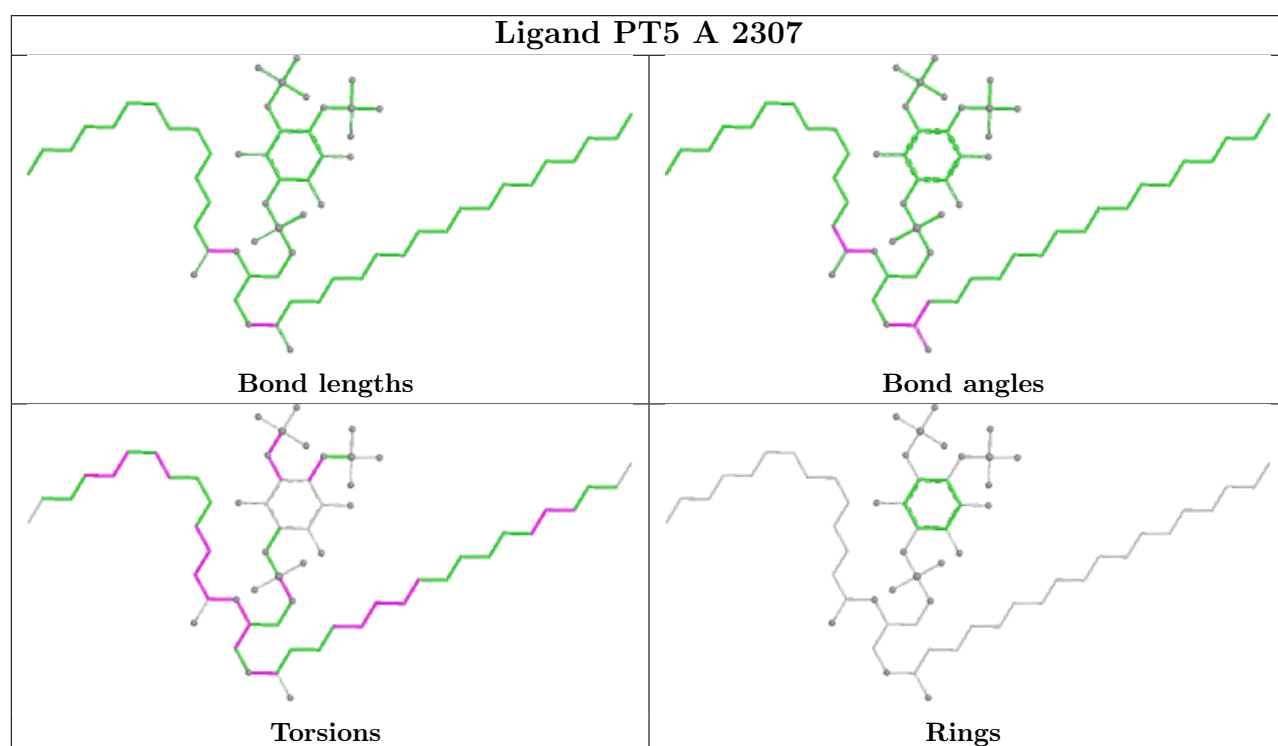
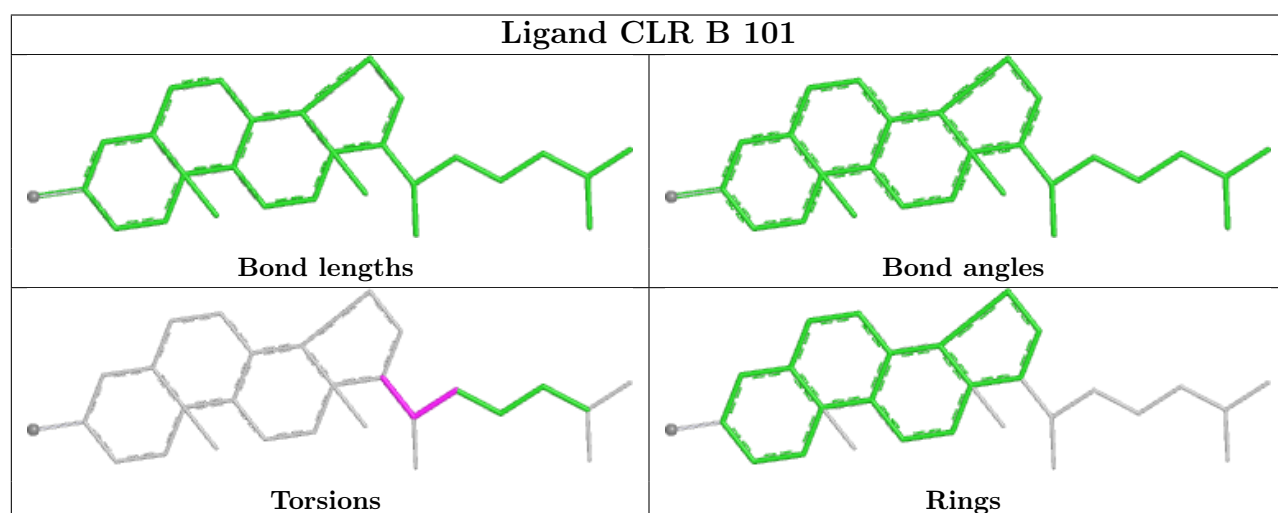
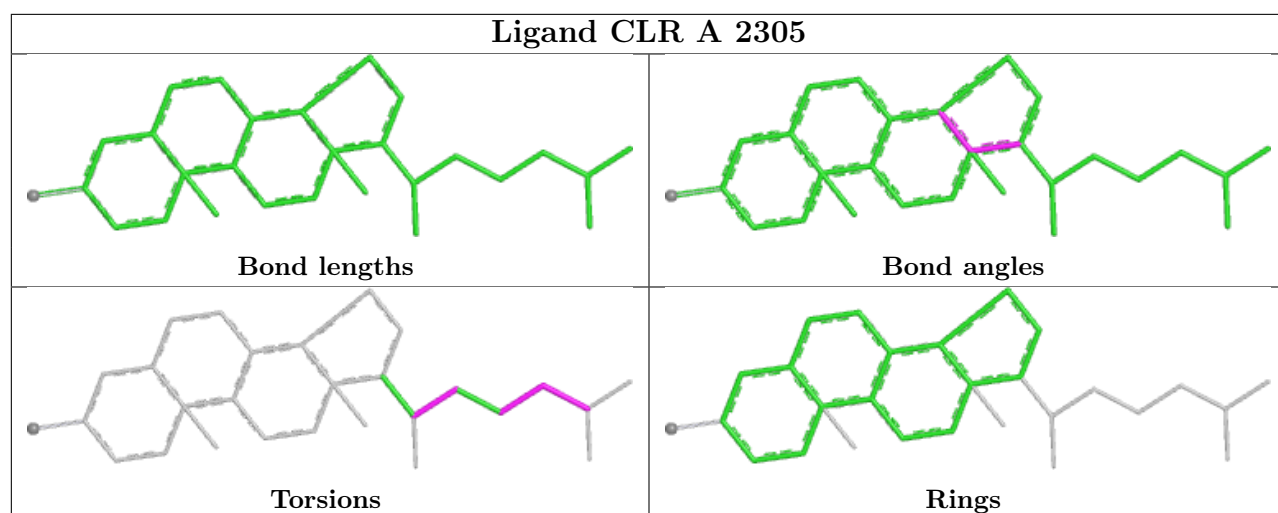
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2305	CLR	1	0
9	B	101	CLR	2	0
11	A	2307	PT5	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

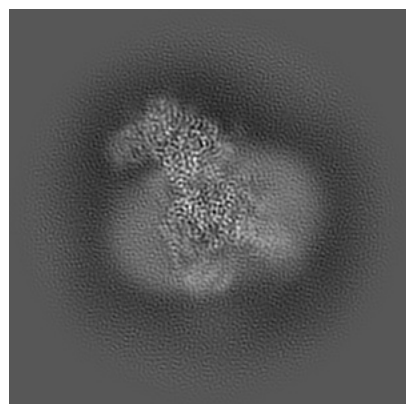
6 Map visualisation [i](#)

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.

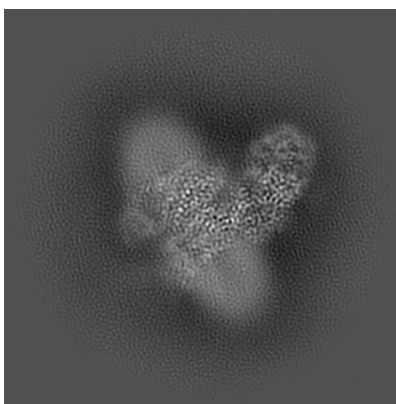
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

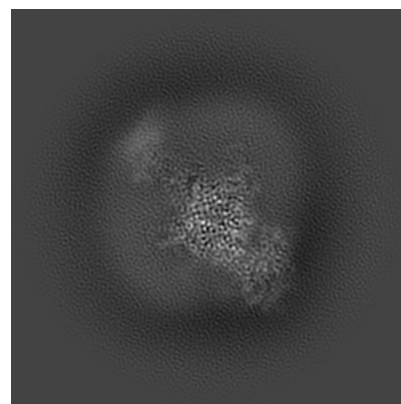
6.1.1 Primary map



X

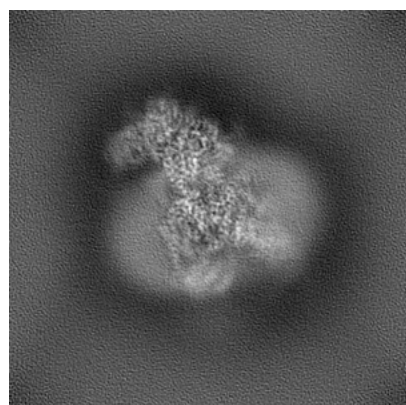


Y

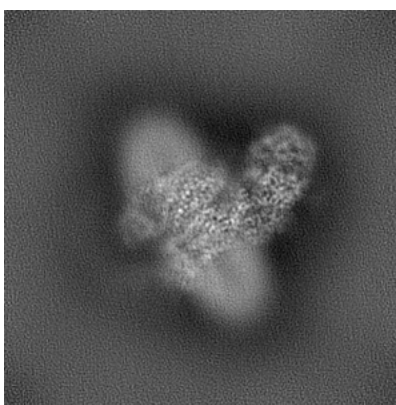


Z

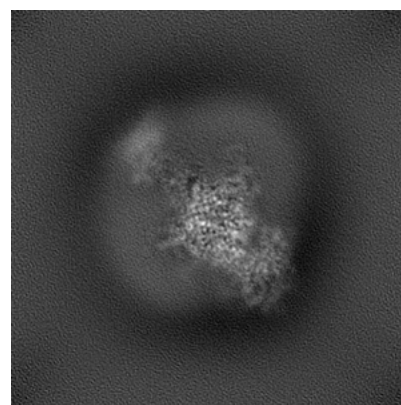
6.1.2 Raw map



X



Y

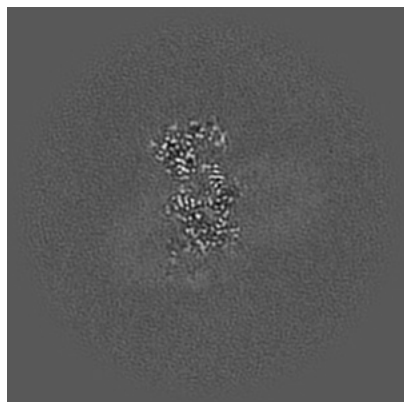


Z

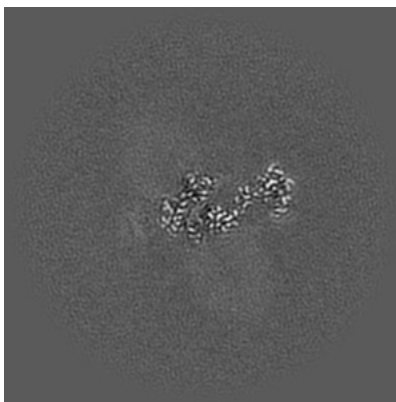
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

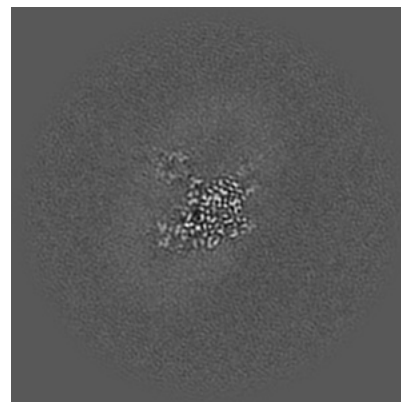
6.2.1 Primary map



X Index: 140

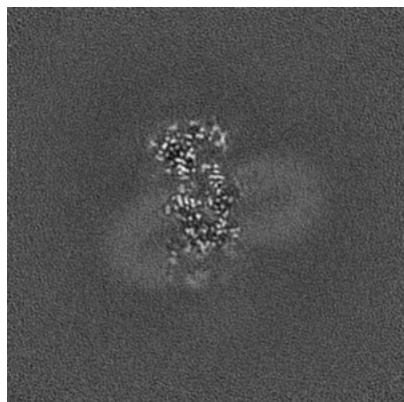


Y Index: 140

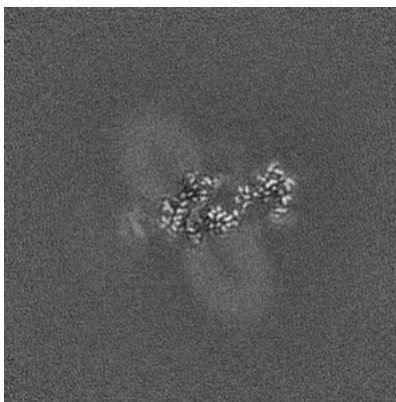


Z Index: 140

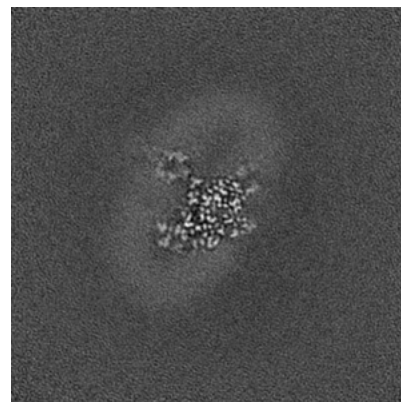
6.2.2 Raw map



X Index: 140



Y Index: 140

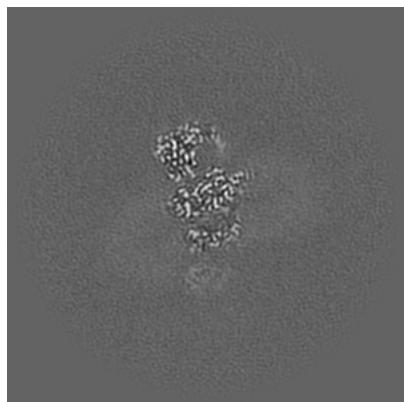


Z Index: 140

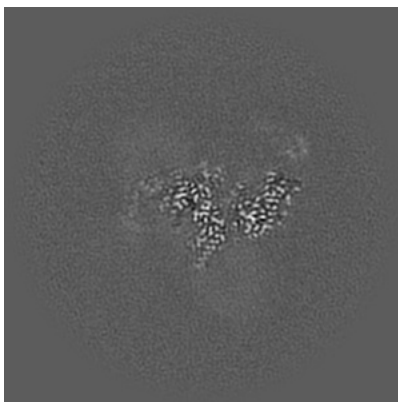
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

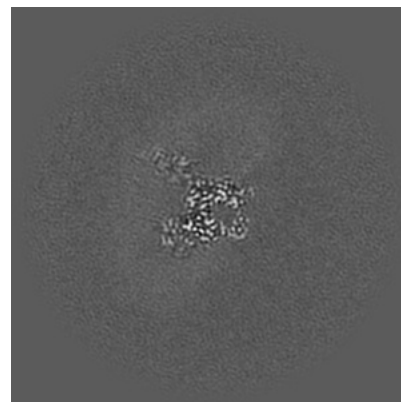
6.3.1 Primary map



X Index: 135

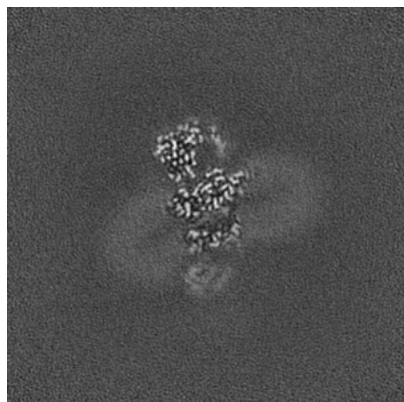


Y Index: 126

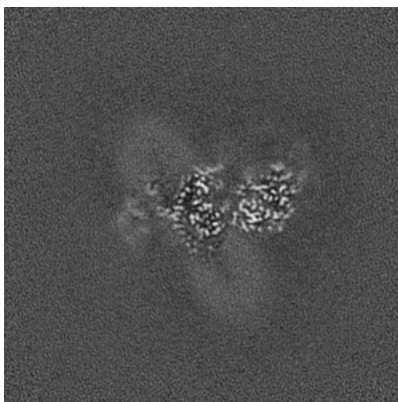


Z Index: 144

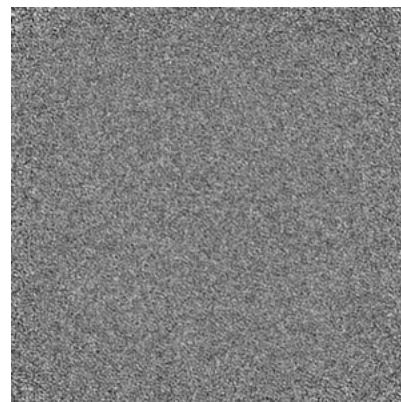
6.3.2 Raw map



X Index: 135



Y Index: 130

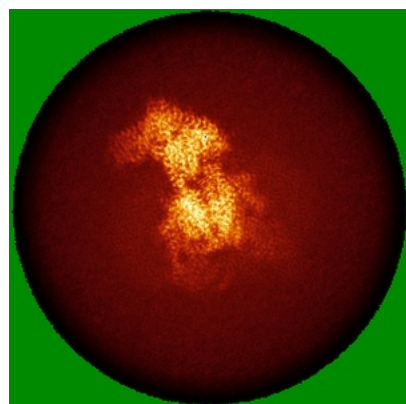


Z Index: 0

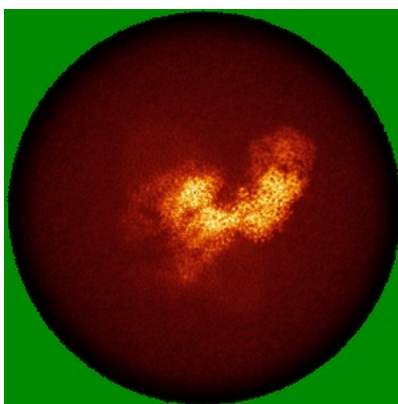
The images above show the largest variance slices of the map in three orthogonal directions.

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

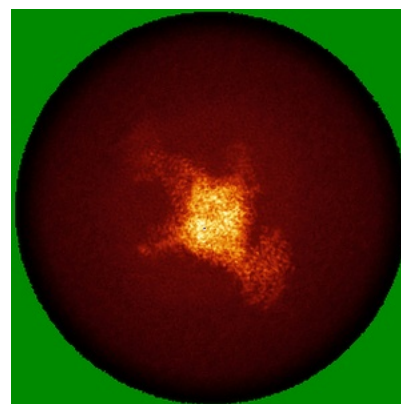
6.4.1 Primary map



X

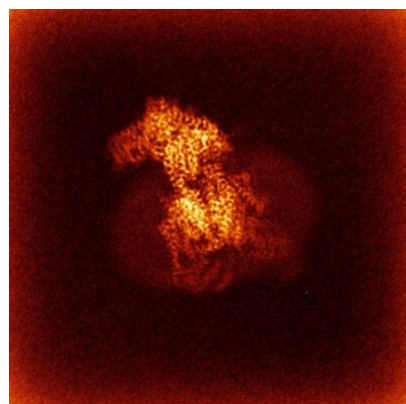


Y

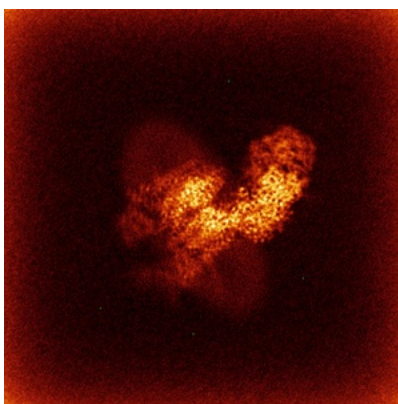


Z

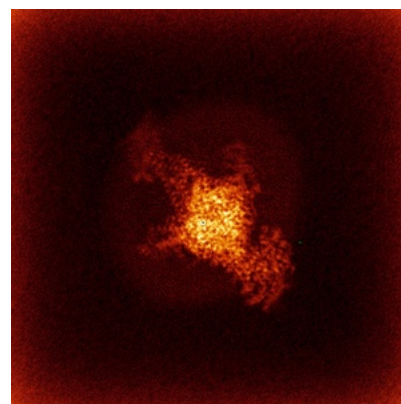
6.4.2 Raw map



X



Y

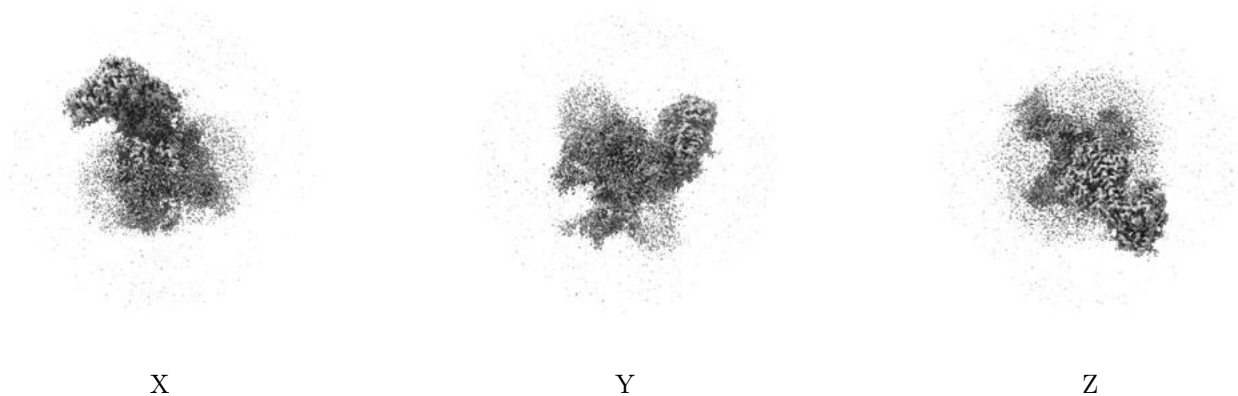


Z

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.

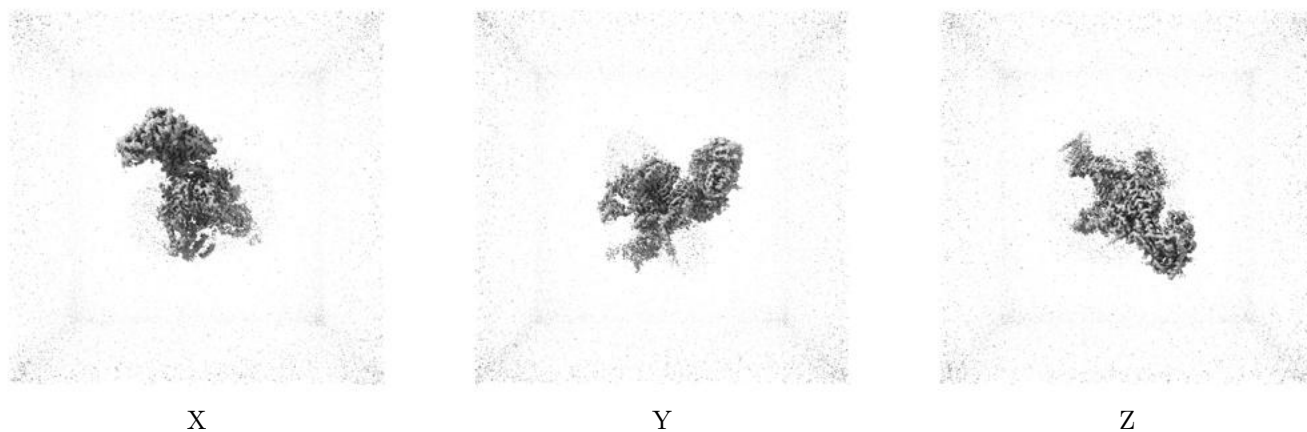
6.5 Orthogonal surface views [i](#)

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.

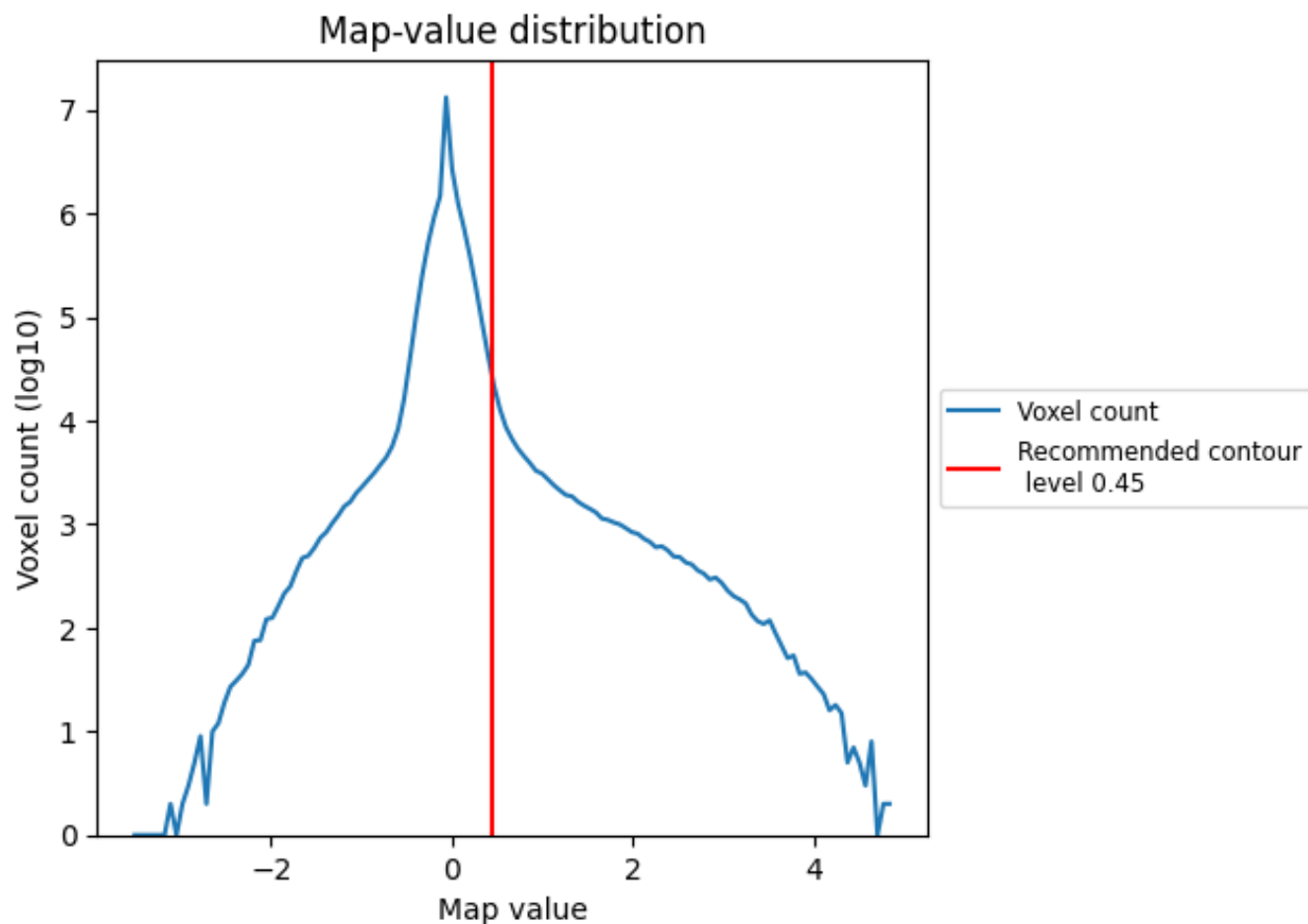
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

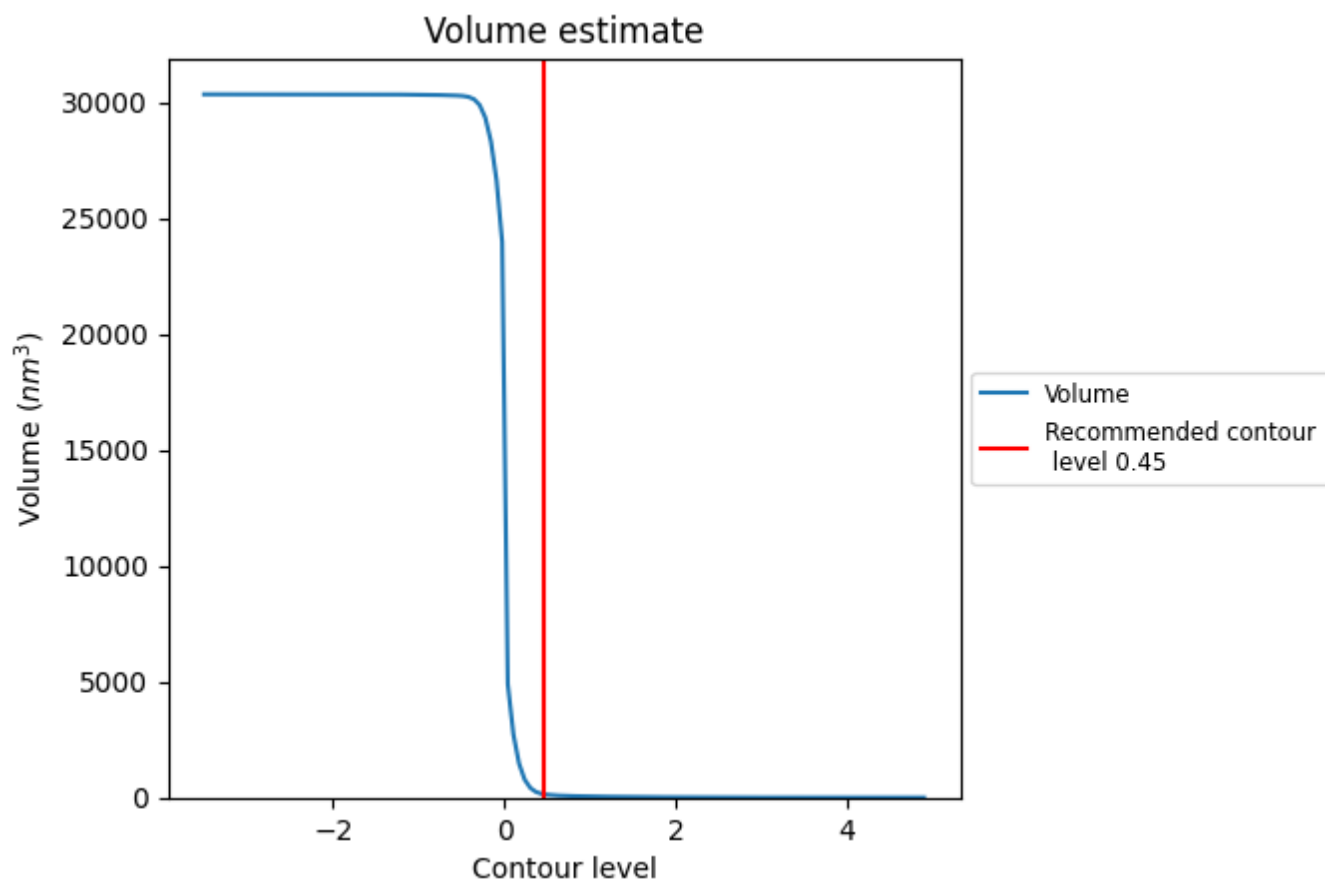
This section contains the results of statistical analysis of the map.

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.

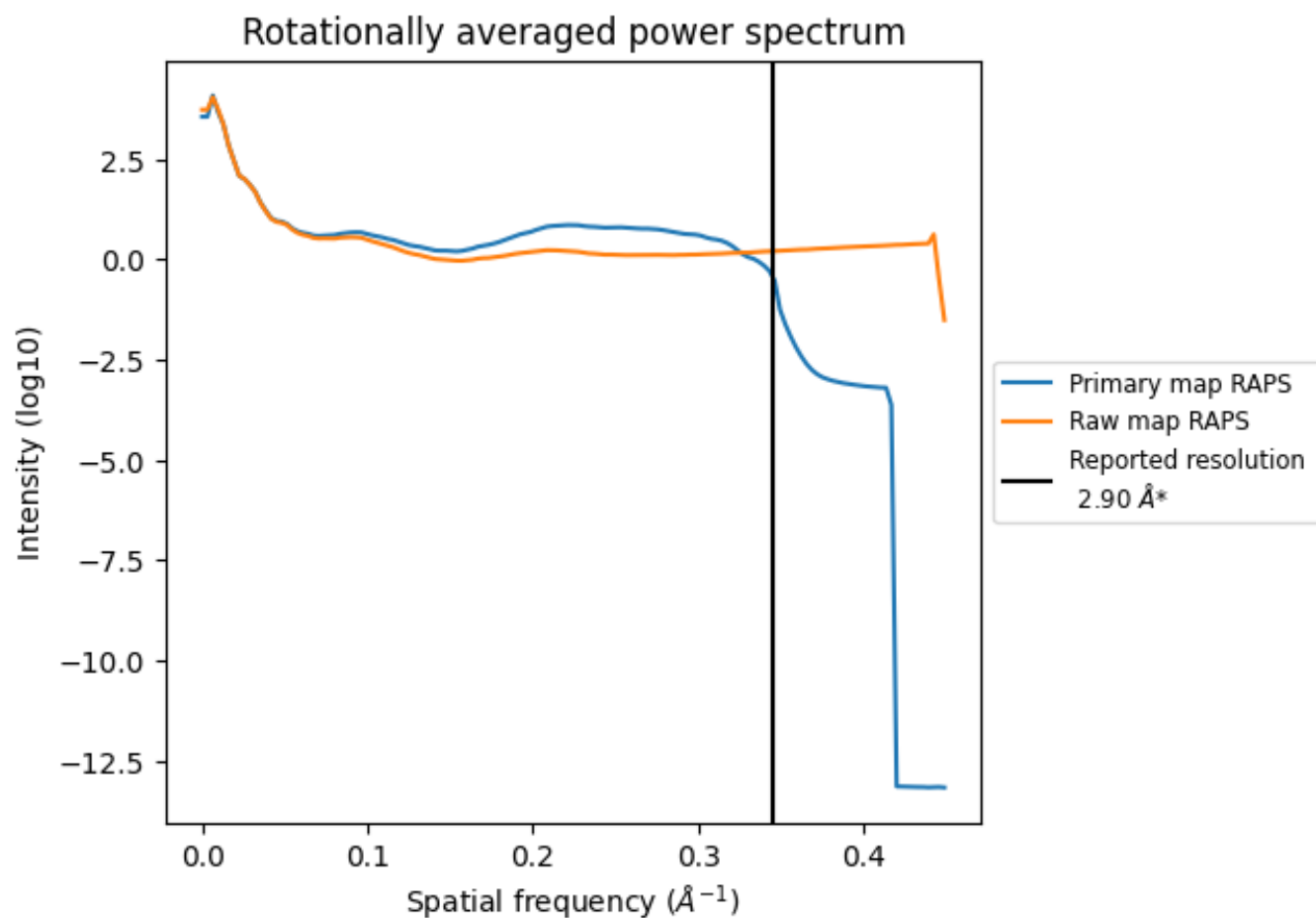
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; 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 ⓘ

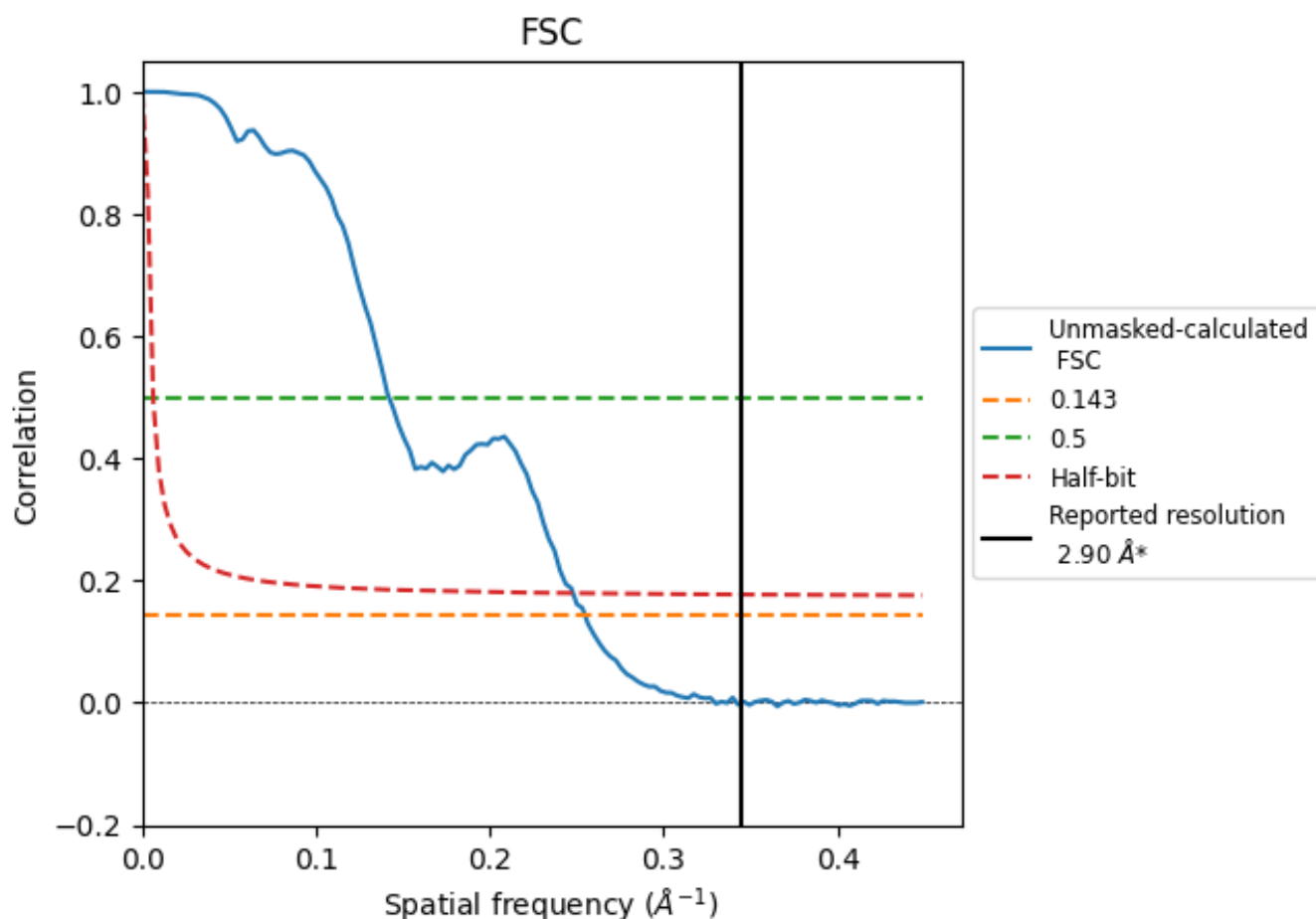


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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

8.2 Resolution estimates [i](#)

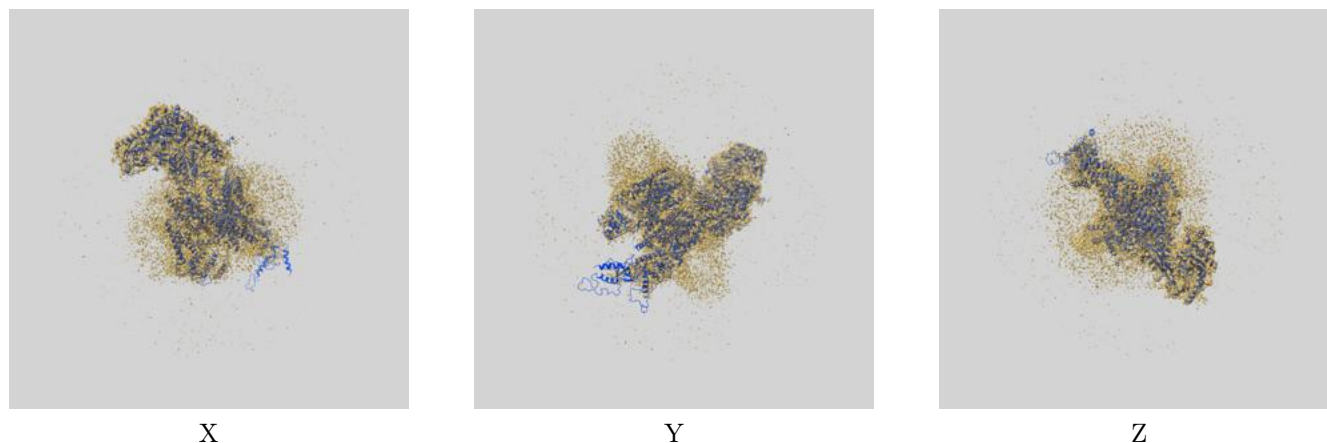
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.05	4.03

*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](#)

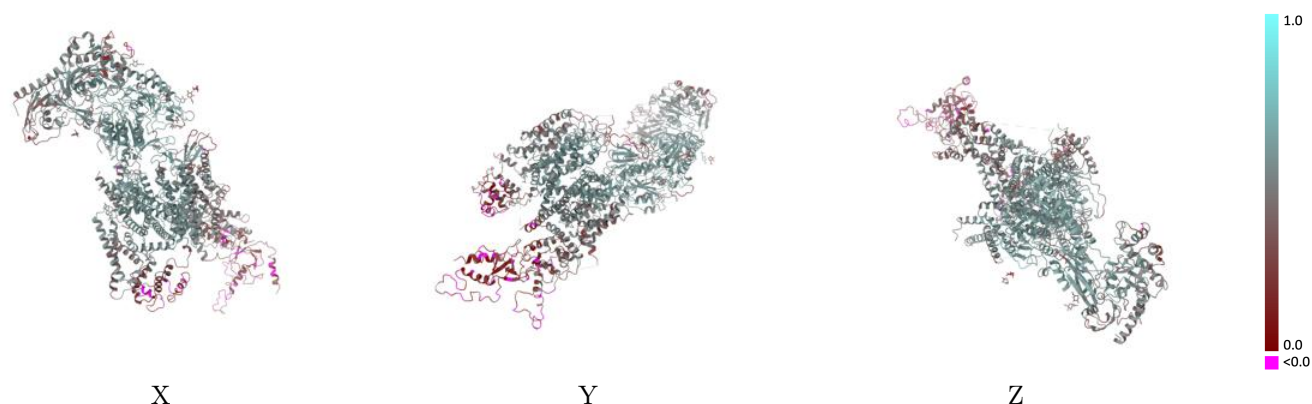
This section contains information regarding the fit between EMDB map EMD-37474 and PDB model 8WE8. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



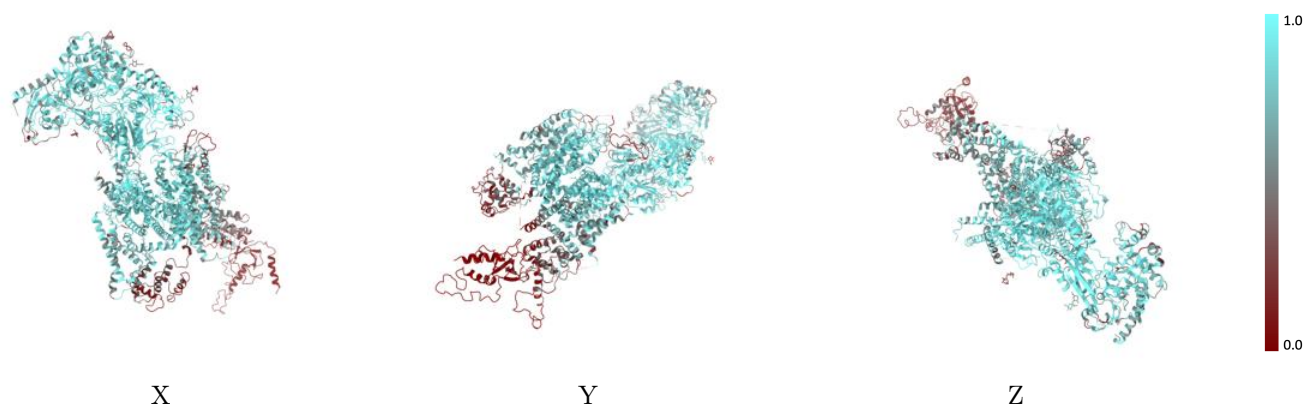
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



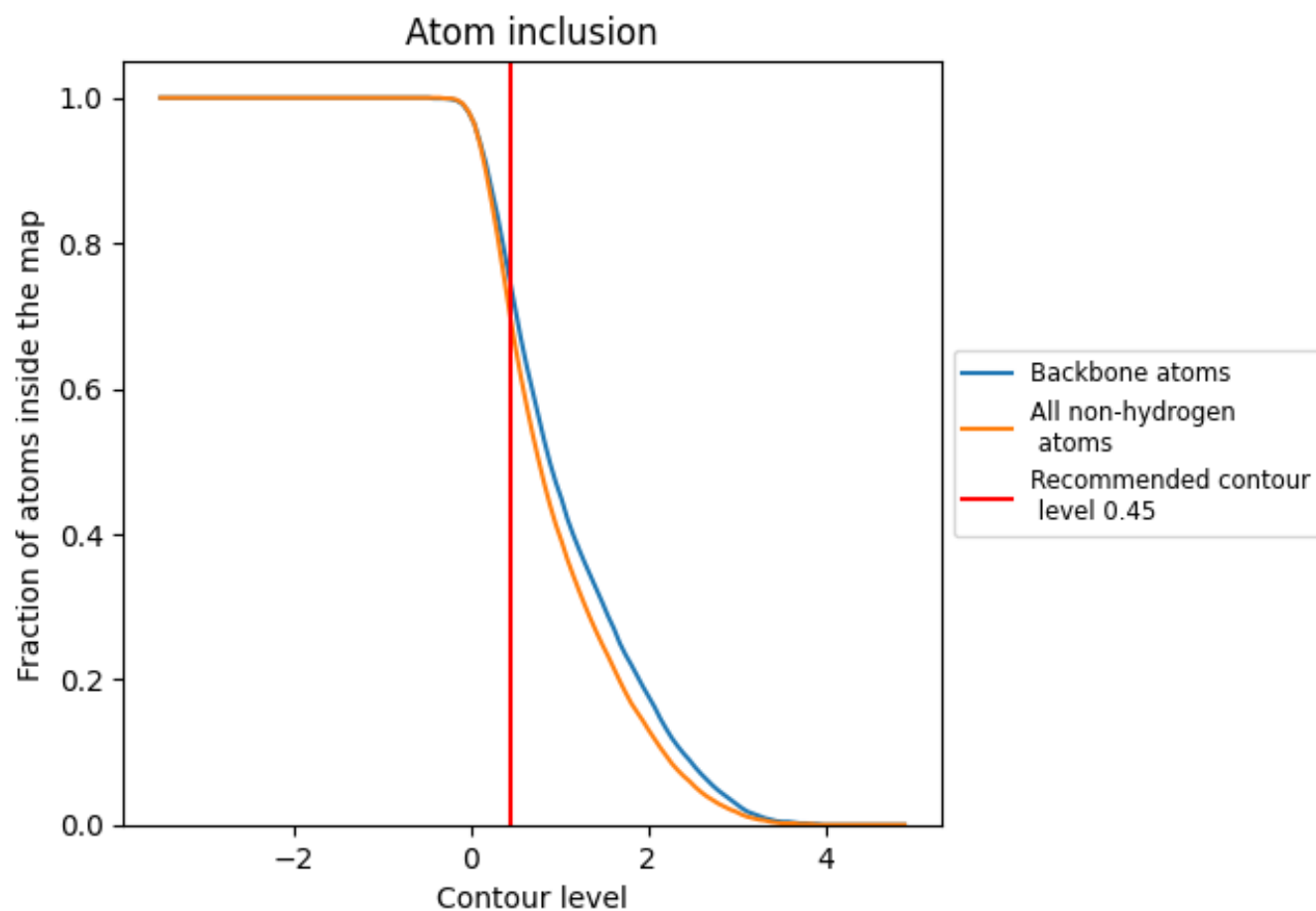
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6950	0.4750
A	0.7370	0.4960
B	0.4100	0.4150
C	0.1690	0.2260
D	0.8380	0.5380
E	0.4760	0.3400
F	0.2500	0.2500
G	0.7500	0.4600
H	0.4290	0.3770
I	0.6070	0.3640

1.0

0.0

<0.0