



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 02:49 AM EST

PDB ID : 8F6P
EMDB ID : EMD-28887
Title : Rat Cardiac Sodium Channel with Ranolazine Bound
Authors : Lenaeus, M.J.; Tonggu, L.
Deposited on : 2022-11-16
Resolution : 3.20 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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

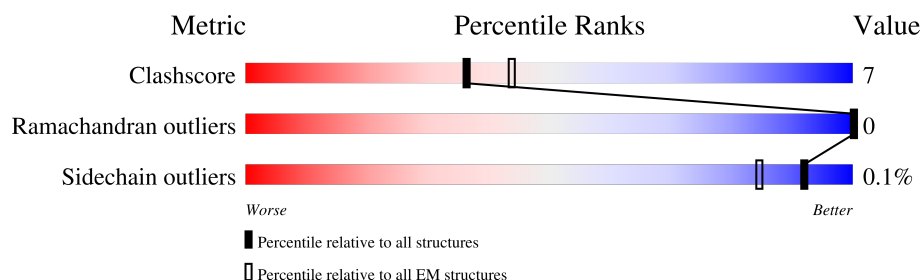
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	1838	
2	B	2	
2	C	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18565 atoms, of which 9287 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 Sodium channel protein type 5 subunit alpha, Green fluorescent protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1091	Total	C	H	N	O	S	0	0
			16596	5535	8229	1341	1431	60		

There are 26 discrepancies between the modelled and reference sequences:

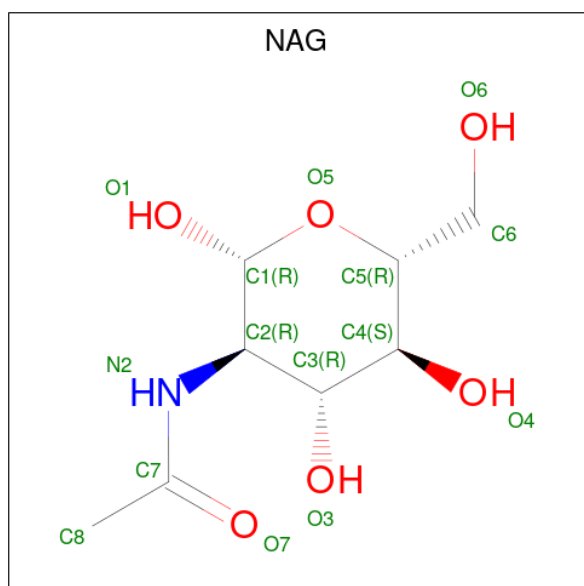
Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLN	GLU	conflict	UNP P15389
A	1499	MET	ALA	conflict	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	1908	MET	-	linker	UNP P15389
A	1909	VAL	-	linker	UNP P15389
A	1972	LEU	PHE	conflict	UNP P42212
A	1973	THR	SER	conflict	UNP P42212
A	2139	LEU	HIS	conflict	UNP P42212
A	2147	GLY	-	expression tag	UNP P42212
A	2148	SER	-	expression tag	UNP P42212
A	2149	ASP	-	expression tag	UNP P42212
A	2150	TYR	-	expression tag	UNP P42212
A	2151	LYS	-	expression tag	UNP P42212
A	2152	ASP	-	expression tag	UNP P42212
A	2153	ASP	-	expression tag	UNP P42212
A	2154	ASP	-	expression tag	UNP P42212
A	2155	ASP	-	expression tag	UNP P42212
A	2156	LYS	-	expression tag	UNP P42212

- Molecule 2 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
2	B	2	Total	C	H	N	O	0	0
			52	16	24	2	10		
2	C	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



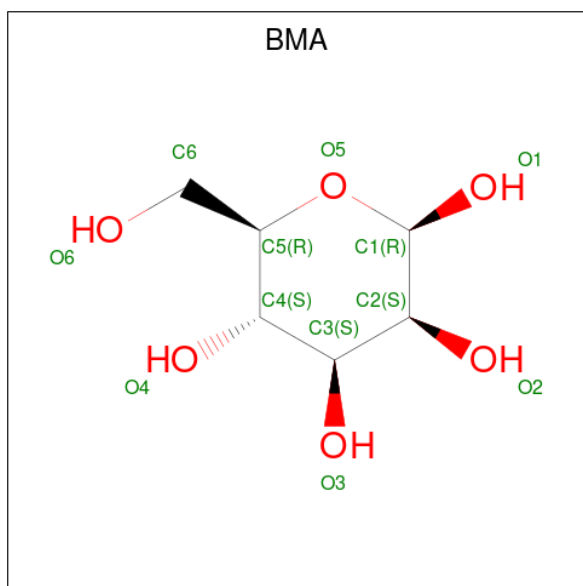
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	N	O
			27	8	13	1	5
3	A	1	Total	C	H	N	O
			26	8	12	1	5
3	A	1	Total	C	H	N	O
			26	8	12	1	5
3	A	1	Total	C	H	N	O
			26	8	12	1	5
3	A	1	Total	C	H	N	O
			27	8	13	1	5
3	A	1	Total	C	H	N	O
			27	8	13	1	5

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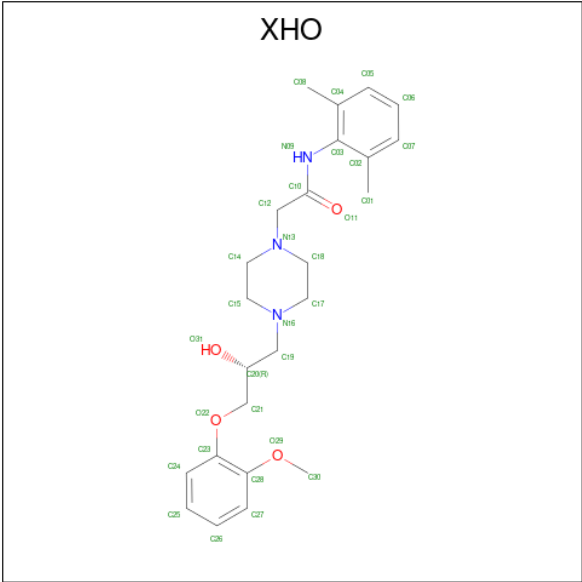
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0

- Molecule 4 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



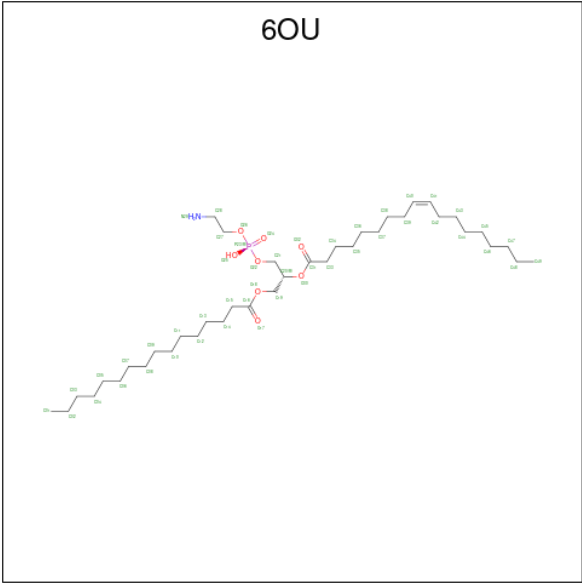
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	21	6	10	5	0
4	A	1	21	6	10	5	0
4	A	1	21	6	10	5	0

- Molecule 5 is (R)-ranolazine (three-letter code: XHO) (formula: $C_{24}H_{33}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			64	24	33	3	4	

- Molecule 6 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P).



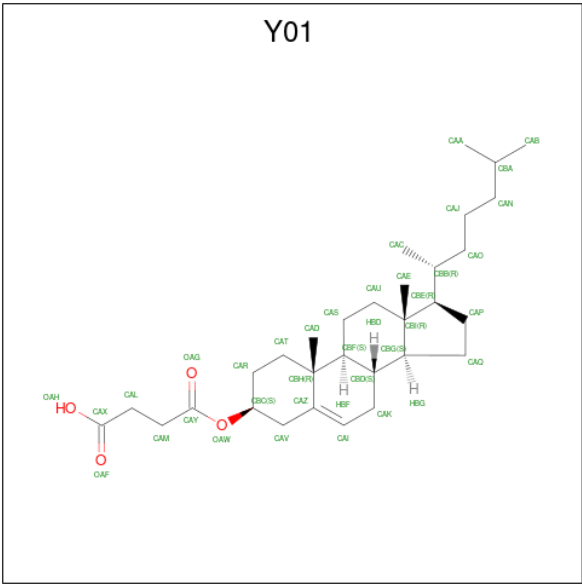
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	0	
			36	26	1	8	1		
6	A	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
6	A	1	Total	C	N	O	P	0	
			41	31	1	8	1		
6	A	1	Total	C	H	N	O	P	0
			108	34	64	1	8	1	
6	A	1	Total	C	H	O	P	0	
			91	29	53	8	1		

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).

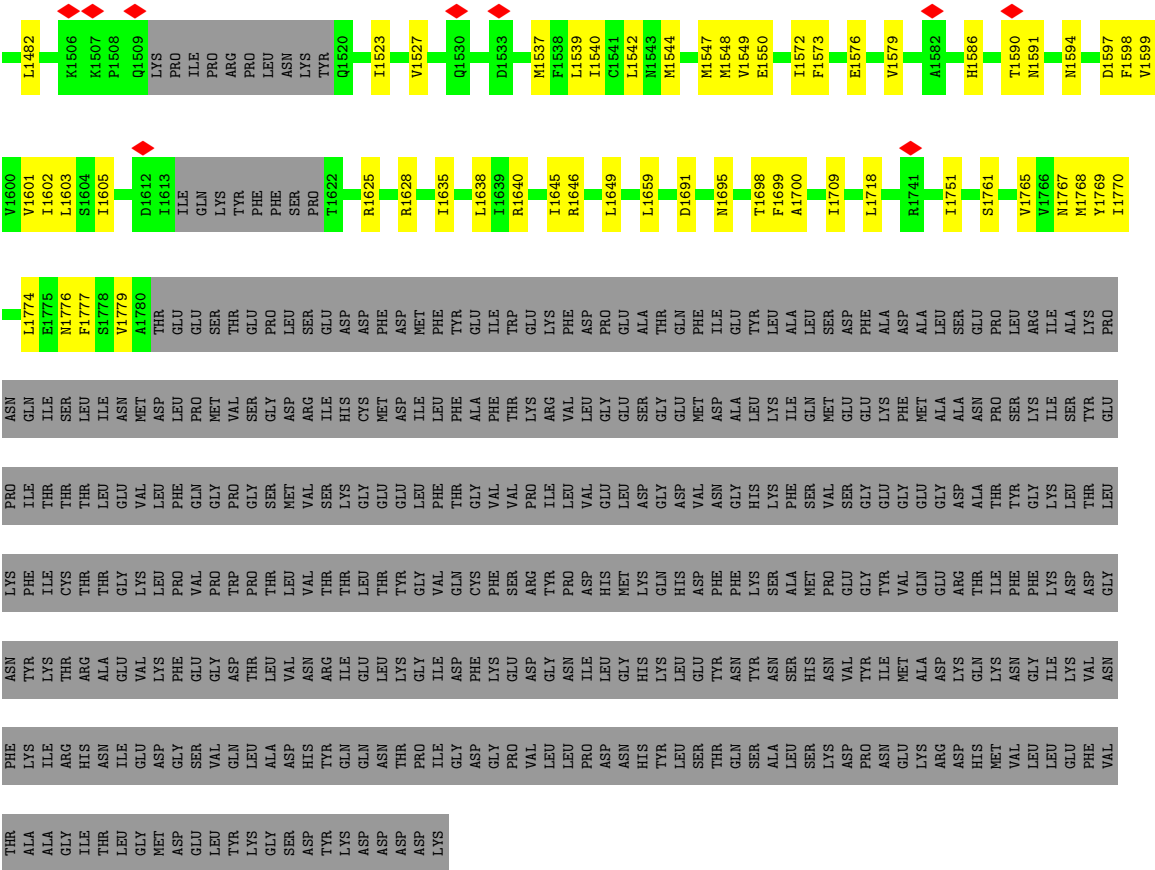


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			73	27	45	1	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			59	23	32	4	
7	A	1	Total	C	H	O	0
			68	27	37	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	

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Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	



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

Chain B: 100%

NAG1
NAG2

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

Chain C: 100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	165532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.173	Depositor
Minimum map value	-2.555	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4171	Depositor
Map size (Å)	270.336, 270.336, 270.336	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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: XHO, Y01, BMA, NAG, 6OU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/8555	0.44	0/11637

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	8367	8229	8245	116	0
2	B	28	24	25	4	0
2	C	28	25	25	0	0
3	A	98	75	91	12	0
4	A	33	30	30	3	0
5	A	31	33	0	1	0
6	A	257	267	0	2	0
7	A	436	604	602	22	0
All	All	9278	9287	9018	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:VAL:HG21	1:A:1285:LEU:HD21	1.65	0.79
1:A:254:VAL:HG21	1:A:412:VAL:HG21	1.70	0.72
1:A:919:LEU:HD21	7:A:2225:Y01:HBG	1.72	0.72
1:A:1601:VAL:O	1:A:1605:ILE:HD12	1.90	0.71
1:A:1381:ASN:OD1	1:A:1434:ARG:NH2	2.24	0.70
1:A:1640:ARG:O	1:A:1646:ARG:NH1	2.24	0.69
1:A:813:LEU:HD21	1:A:1352:ILE:HG21	1.74	0.69
5:A:2211:XHO:O31	5:A:2211:XHO:O29	2.11	0.68
1:A:1376:ASN:OD1	3:A:2208:NAG:N2	2.28	0.67
1:A:1765:VAL:O	1:A:1769:TYR:HB3	1.94	0.67
1:A:1482:LEU:HD23	1:A:1482:LEU:O	1.96	0.65
7:A:2218:Y01:HAC3	7:A:2218:Y01:HAN2	1.77	0.65
1:A:1397:TRP:H	2:B:1:NAG:H83	1.61	0.63
1:A:254:VAL:CG2	1:A:412:VAL:HG21	2.28	0.62
1:A:244:LEU:HD11	1:A:932:VAL:HG22	1.81	0.62
7:A:2219:Y01:HAD2	7:A:2221:Y01:HAU1	1.81	0.61
1:A:1761:SER:O	1:A:1765:VAL:HG22	2.00	0.61
3:A:2201:NAG:C1	3:A:2201:NAG:H82	2.30	0.61
1:A:913:SER:OG	1:A:914:GLY:N	2.33	0.61
1:A:197:LEU:O	1:A:201:VAL:HG23	2.00	0.61
3:A:2208:NAG:C1	3:A:2208:NAG:H82	2.30	0.61
1:A:373:ASP:OD2	1:A:903:ILE:HG22	2.01	0.60
1:A:886:ASP:OD1	1:A:887:PHE:N	2.34	0.60
1:A:840:LEU:HD12	1:A:940:LEU:HD12	1.84	0.59
3:A:2202:NAG:H82	3:A:2202:NAG:C1	2.32	0.59
1:A:1659:LEU:HD22	1:A:1769:TYR:CD1	2.36	0.59
1:A:1691:ASP:O	1:A:1695:ASN:ND2	2.35	0.58
1:A:840:LEU:HD11	1:A:939:ALA:HB1	1.85	0.58
1:A:1344:LEU:HD11	7:A:2221:Y01:HAM1	1.85	0.57
7:A:2222:Y01:HAE2	7:A:2222:Y01:HAC1	1.86	0.57
1:A:1550:GLU:OE2	1:A:1628:ARG:NH2	2.39	0.56
1:A:1599:VAL:O	1:A:1603:LEU:HD23	2.06	0.56
1:A:919:LEU:HD11	7:A:2225:Y01:HAK2	1.87	0.55
1:A:1547:MET:CE	1:A:1635:ILE:HD11	2.35	0.55
4:A:2206:BMA:O2	2:B:2:NAG:H83	2.08	0.54
3:A:2208:NAG:C1	3:A:2208:NAG:C8	2.86	0.54
1:A:1709:ILE:HG21	1:A:1718:LEU:HD12	1.90	0.54
1:A:166:THR:O	1:A:170:THR:OG1	2.19	0.53
1:A:1700:ALA:HB1	7:A:2222:Y01:HAP1	1.89	0.53
1:A:271:GLN:O	1:A:1625:ARG:NH1	2.41	0.53
1:A:1253:VAL:O	1:A:1257:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2201:NAG:C1	3:A:2201:NAG:C8	2.86	0.53
7:A:2226:Y01:HAE2	7:A:2226:Y01:HAC1	1.91	0.53
1:A:1244:ALA:O	1:A:1248:PHE:CD1	2.61	0.53
1:A:1423:TRP:HE3	1:A:1427:MET:SD	2.32	0.53
1:A:1455:PHE:O	1:A:1459:GLY:N	2.40	0.53
1:A:1329:LEU:HD13	1:A:1768:MET:CE	2.39	0.52
1:A:284:ASN:OD1	1:A:284:ASN:N	2.29	0.52
1:A:1542:LEU:HD21	7:A:2223:Y01:HAL2	1.92	0.52
1:A:1776:ASN:HA	1:A:1779:VAL:HG22	1.92	0.52
1:A:399:PHE:O	1:A:400:LEU:HD23	2.11	0.51
3:A:2202:NAG:C1	3:A:2202:NAG:C8	2.88	0.51
1:A:919:LEU:HD21	7:A:2225:Y01:HAK2	1.91	0.51
1:A:1549:VAL:HG12	1:A:1549:VAL:O	2.11	0.51
1:A:1404:PHE:CE1	1:A:1413:ALA:HB3	2.46	0.50
1:A:906:MET:O	1:A:910:MET:HG3	2.11	0.50
1:A:1423:TRP:CE3	1:A:1427:MET:SD	3.04	0.50
1:A:1381:ASN:O	1:A:1434:ARG:NH2	2.45	0.50
1:A:1659:LEU:HD13	1:A:1769:TYR:HE1	1.75	0.50
1:A:366:LEU:CD2	1:A:369:LEU:HD12	2.42	0.50
1:A:1307:LEU:HD11	1:A:1310:LEU:HD12	1.95	0.49
1:A:1345:ILE:HD11	7:A:2218:Y01:HAC2	1.94	0.49
1:A:1227:GLU:HA	1:A:1231:LEU:HD11	1.94	0.49
1:A:1350:PHE:O	1:A:1451:TYR:OH	2.31	0.49
1:A:1282:ASP:O	1:A:1286:VAL:HG23	2.13	0.49
1:A:1355:VAL:O	1:A:1359:ALA:HB2	2.13	0.49
1:A:1329:LEU:HD13	1:A:1768:MET:HE1	1.95	0.48
1:A:1751:ILE:HD13	6:A:2214:6OU:O32	2.14	0.48
1:A:233:VAL:HG22	1:A:233:VAL:O	2.14	0.48
1:A:224:VAL:HG11	1:A:857:VAL:HG23	1.96	0.47
1:A:927:VAL:HG21	7:A:2226:Y01:HAM1	1.96	0.47
1:A:1544:MET:O	1:A:1548:MET:HG3	2.15	0.47
1:A:270:LEU:O	1:A:274:MET:HB2	2.14	0.46
1:A:242:GLY:O	1:A:246:GLN:OE1	2.33	0.46
1:A:219:LEU:HD12	1:A:222:PHE:HD2	1.80	0.46
1:A:737:LEU:HD13	7:A:2219:Y01:HAK2	1.97	0.46
1:A:762:THR:HG22	1:A:790:VAL:CG2	2.46	0.46
4:A:2207:BMA:HO4	4:A:2207:BMA:HO6	1.58	0.46
1:A:361:TRP:HE1	7:A:2225:Y01:HAA2	1.80	0.46
1:A:1214:ILE:O	1:A:1218:LEU:HD13	2.16	0.46
1:A:1376:ASN:OD1	3:A:2208:NAG:C2	2.63	0.46
1:A:1539:LEU:HD23	1:A:1572:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:O	1:A:415:MET:HG2	2.16	0.45
4:A:2204:BMA:C1	2:B:2:NAG:HO3	2.29	0.45
1:A:746:PHE:O	1:A:750:LEU:HD23	2.16	0.45
1:A:1537:MET:O	1:A:1540:ILE:HG22	2.15	0.45
1:A:1427:MET:O	1:A:1431:VAL:HG22	2.16	0.45
1:A:1586:HIS:O	1:A:1590:THR:N	2.49	0.45
1:A:354:THR:O	1:A:354:THR:HG23	2.16	0.45
1:A:1523:ILE:O	1:A:1527:VAL:HG22	2.17	0.45
1:A:737:LEU:HD13	7:A:2219:Y01:CAK	2.47	0.45
1:A:1351:SER:O	1:A:1355:VAL:HG23	2.16	0.45
6:A:2216:6OU:C39	7:A:2222:Y01:HAE3	2.47	0.44
1:A:256:VAL:HG12	1:A:1645:ILE:HD11	1.99	0.44
1:A:309:LEU:HD13	1:A:345:ALA:CB	2.48	0.44
1:A:415:MET:O	1:A:419:GLU:HG2	2.18	0.44
7:A:2218:Y01:HAA1	7:A:2218:Y01:HBB	2.00	0.44
1:A:1339:VAL:CG2	1:A:1470:VAL:HG11	2.48	0.43
1:A:1365:CYS:SG	1:A:1380:VAL:HG11	2.59	0.43
3:A:2201:NAG:H83	3:A:2201:NAG:H3	1.99	0.43
1:A:415:MET:HG3	1:A:1777:PHE:HE2	1.84	0.43
1:A:1540:ILE:HG23	1:A:1638:LEU:HD21	2.00	0.43
1:A:1591:ASN:OD1	1:A:1594:ASN:N	2.49	0.43
1:A:364:LEU:HD13	7:A:2225:Y01:HAI	1.99	0.43
1:A:1471:ILE:HG21	1:A:1767:ASN:HB3	2.01	0.43
1:A:897:ILE:HD11	1:A:922:PHE:CE2	2.54	0.43
1:A:1659:LEU:HD22	1:A:1769:TYR:HD1	1.77	0.43
1:A:1770:ILE:O	1:A:1774:LEU:HD13	2.18	0.43
3:A:2202:NAG:H83	3:A:2202:NAG:H3	2.00	0.43
1:A:1573:PHE:O	1:A:1576:GLU:HG3	2.19	0.42
1:A:1310:LEU:HD22	1:A:1313:LEU:CD1	2.49	0.42
1:A:322:THR:HG22	1:A:322:THR:O	2.18	0.42
1:A:1597:ASP:O	1:A:1601:VAL:HG23	2.20	0.42
1:A:329:ASN:OD1	3:A:2202:NAG:O5	2.38	0.42
1:A:373:ASP:OD1	1:A:901:GLU:HA	2.20	0.42
1:A:1544:MET:HB2	1:A:1635:ILE:HD12	2.01	0.42
1:A:1698:THR:HG22	1:A:1699:PHE:N	2.34	0.42
1:A:922:PHE:HA	1:A:925:VAL:HG12	2.02	0.42
1:A:1576:GLU:HA	1:A:1579:VAL:HG22	2.02	0.42
1:A:373:ASP:OD2	1:A:903:ILE:CG2	2.67	0.41
7:A:2224:Y01:HAE2	7:A:2224:Y01:HAC1	2.01	0.41
1:A:146:CYS:HA	1:A:149:MET:HE2	2.01	0.41
3:A:2208:NAG:H3	3:A:2208:NAG:H83	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2228:Y01:HAR2	7:A:2228:Y01:OAG	2.20	0.41
1:A:155:PRO:HG2	1:A:158:THR:HG23	2.01	0.41
1:A:757:PHE:O	1:A:760:ILE:HG22	2.20	0.41
1:A:1598:PHE:O	1:A:1602:ILE:HG12	2.20	0.41
1:A:1645:ILE:O	1:A:1649:LEU:HD23	2.20	0.41
1:A:360:ALA:CB	7:A:2225:Y01:HAE2	2.50	0.41
1:A:360:ALA:HB1	7:A:2225:Y01:CAE	2.50	0.41
1:A:288:LEU:HD21	1:A:296:GLU:CB	2.50	0.41
1:A:410:LEU:HD22	1:A:934:LEU:CD1	2.51	0.41
1:A:1248:PHE:HA	1:A:1251:VAL:HG12	2.02	0.41
1:A:1397:TRP:N	2:B:1:NAG:H83	2.33	0.41
1:A:1447:TYR:HB3	1:A:1450:ILE:HD12	2.03	0.40
1:A:419:GLU:OE2	1:A:419:GLU:HA	2.21	0.40
1:A:733:LEU:O	1:A:737:LEU:HD23	2.21	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	1075/1838 (58%)	1036 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	850/1613 (53%)	849 (100%)	1 (0%)	92 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	ASN

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

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 ⓘ

4 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	$\# Z > 2$
2	NAG	B	1	2	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	B	2	2	14,14,15	0.45	0	17,19,21	0.43	0
2	NAG	C	1	2,1	14,14,15	0.29	0	17,19,21	0.54	0
2	NAG	C	2	2	14,14,15	0.54	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
2	NAG	B	1	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

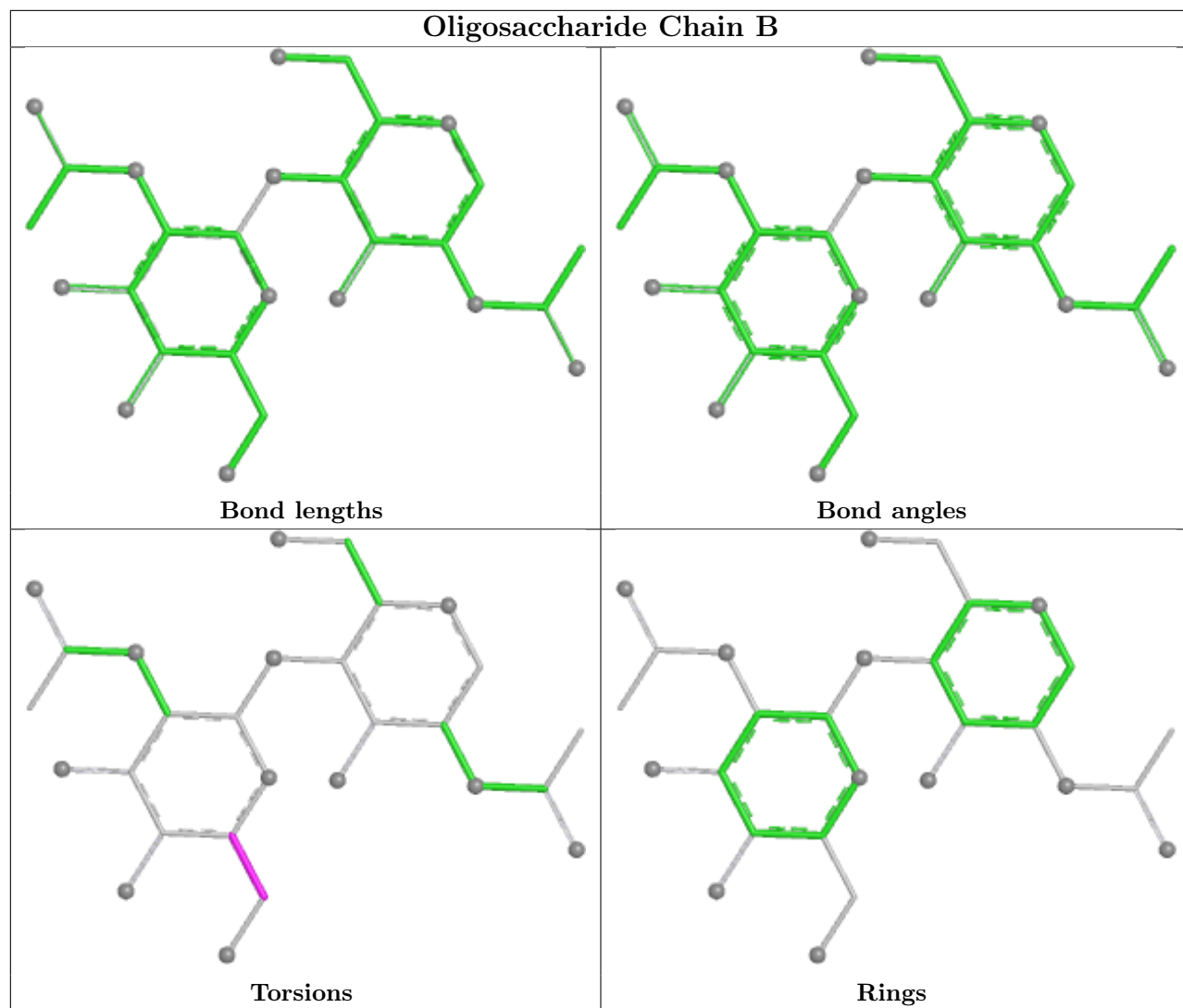
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

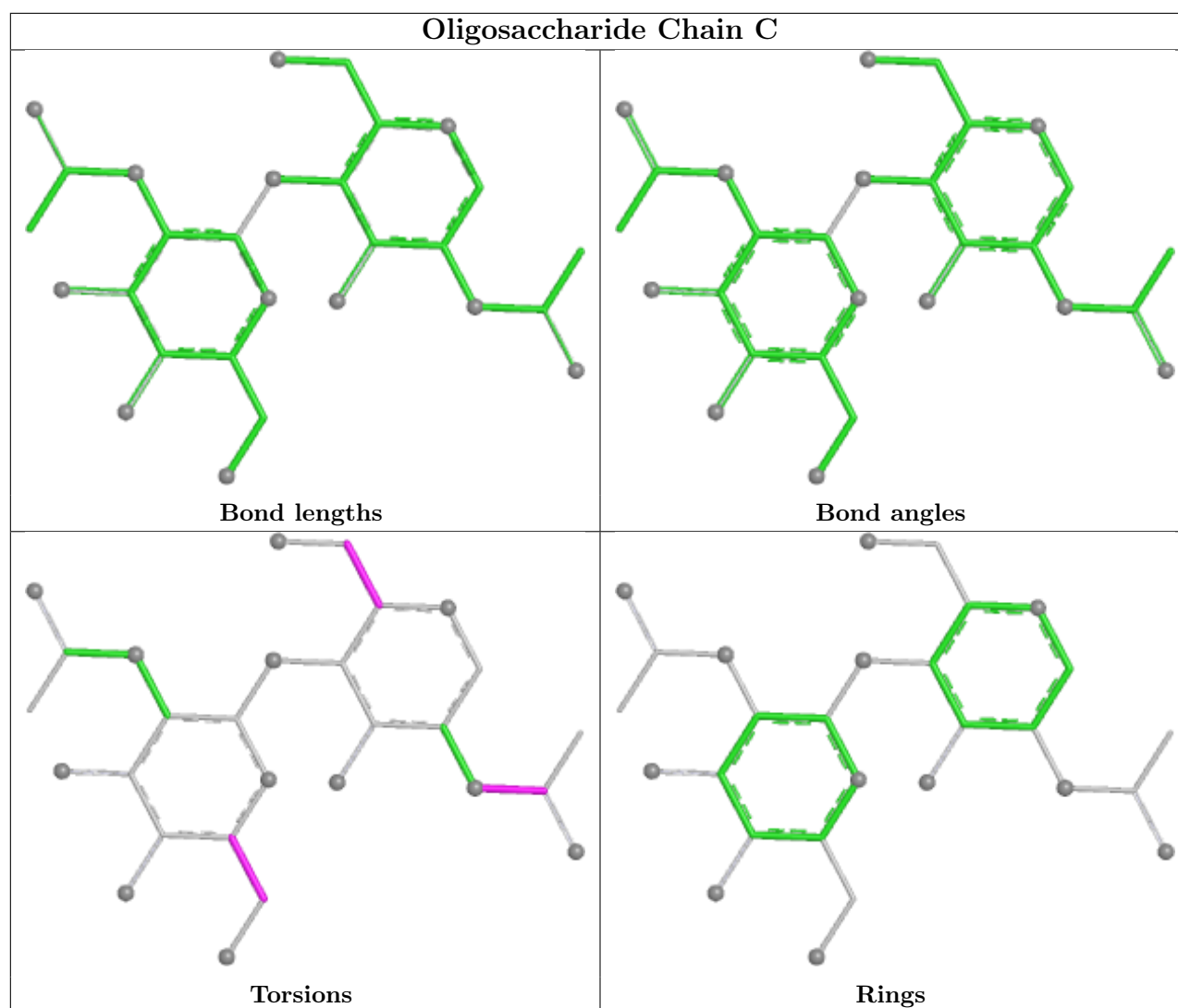
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	B	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

30 ligands 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	$\# Z > 2$
7	Y01	A	2221	-	34,34,38	1.44	5 (14%)	49,51,57	2.15	13 (26%)
6	6OU	A	2214	-	48,48,48	1.40	7 (14%)	51,53,53	1.29	3 (5%)
7	Y01	A	2227	-	38,38,38	1.28	4 (10%)	57,57,57	2.08	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	Y01	A	2229	-	38,38,38	3.24	19 (50%)	57,57,57	3.02	24 (42%)
7	Y01	A	2218	-	31,31,38	1.21	3 (9%)	48,48,57	1.82	6 (12%)
7	Y01	A	2226	-	38,38,38	1.22	3 (7%)	57,57,57	2.05	12 (21%)
7	Y01	A	2225	-	38,38,38	1.35	4 (10%)	57,57,57	2.02	12 (21%)
6	6OU	A	2216	-	43,43,48	1.46	7 (16%)	46,48,53	1.28	3 (6%)
3	NAG	A	2202	-	14,14,15	0.37	0	17,19,21	1.25	2 (11%)
7	Y01	A	2220	-	30,30,38	1.39	4 (13%)	46,46,57	2.14	8 (17%)
7	Y01	A	2223	-	38,38,38	1.24	3 (7%)	57,57,57	1.98	10 (17%)
6	6OU	A	2212	-	35,35,48	1.59	7 (20%)	38,40,53	1.34	4 (10%)
3	NAG	A	2210	-	14,14,15	0.21	0	17,19,21	0.44	0
5	XHO	A	2211	-	33,33,33	1.17	3 (9%)	44,44,44	1.41	7 (15%)
7	Y01	A	2219	-	38,38,38	1.27	4 (10%)	57,57,57	1.99	10 (17%)
4	BMA	A	2204	-	11,11,12	0.82	0	15,15,17	0.86	0
3	NAG	A	2201	1	14,14,15	0.24	0	17,19,21	0.85	1 (5%)
4	BMA	A	2206	-	11,11,12	0.54	0	15,15,17	0.75	0
3	NAG	A	2208	1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
4	BMA	A	2207	-	11,11,12	0.49	0	15,15,17	0.89	0
6	6OU	A	2213	-	48,48,48	1.41	7 (14%)	51,53,53	1.23	4 (7%)
7	Y01	A	2222	-	38,38,38	1.35	4 (10%)	57,57,57	2.04	15 (26%)
6	6OU	A	2217	-	37,37,48	1.51	7 (18%)	40,42,53	1.09	2 (5%)
7	Y01	A	2230	-	38,38,38	1.27	4 (10%)	57,57,57	2.01	11 (19%)
3	NAG	A	2205	-	14,14,15	0.19	0	17,19,21	0.42	0
6	6OU	A	2215	-	40,40,48	1.48	7 (17%)	43,45,53	1.17	3 (6%)
7	Y01	A	2228	-	38,38,38	1.25	3 (7%)	57,57,57	1.95	10 (17%)
3	NAG	A	2203	-	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	A	2209	-	14,14,15	0.21	0	17,19,21	0.46	0
7	Y01	A	2224	-	38,38,38	1.28	4 (10%)	57,57,57	2.01	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	Y01	A	2221	-	-	3/13/71/77	0/4/4/4
6	6OU	A	2214	-	-	21/52/52/52	-
7	Y01	A	2227	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	Y01	A	2229	-	-	14/19/77/77	0/4/4/4
7	Y01	A	2218	-	-	5/10/68/77	0/4/4/4
7	Y01	A	2226	-	-	9/19/77/77	0/4/4/4
7	Y01	A	2225	-	-	5/19/77/77	0/4/4/4
6	6OU	A	2216	-	-	25/47/47/52	-
3	NAG	A	2202	-	-	4/6/23/26	0/1/1/1
7	Y01	A	2220	-	-	6/9/63/77	0/4/4/4
7	Y01	A	2223	-	-	9/19/77/77	0/4/4/4
6	6OU	A	2212	-	-	14/39/39/52	-
3	NAG	A	2210	-	-	4/6/23/26	0/1/1/1
5	XHO	A	2211	-	-	9/19/29/29	0/3/3/3
7	Y01	A	2219	-	-	7/19/77/77	0/4/4/4
4	BMA	A	2204	-	-	0/2/19/22	0/1/1/1
3	NAG	A	2201	1	-	5/6/23/26	0/1/1/1
4	BMA	A	2206	-	-	0/2/19/22	0/1/1/1
3	NAG	A	2208	1	-	5/6/23/26	0/1/1/1
4	BMA	A	2207	-	-	1/2/19/22	1/1/1/1
6	6OU	A	2213	-	-	21/52/52/52	-
7	Y01	A	2222	-	-	5/19/77/77	0/4/4/4
6	6OU	A	2217	-	-	19/41/41/52	-
7	Y01	A	2230	-	-	5/19/77/77	0/4/4/4
3	NAG	A	2205	-	-	1/6/23/26	0/1/1/1
6	6OU	A	2215	-	-	26/44/44/52	-
7	Y01	A	2228	-	-	8/19/77/77	0/4/4/4
3	NAG	A	2203	-	-	0/6/23/26	0/1/1/1
3	NAG	A	2209	-	-	4/6/23/26	0/1/1/1
7	Y01	A	2224	-	-	10/19/77/77	0/4/4/4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2229	Y01	CAL-CAX	7.01	1.66	1.50
7	A	2229	Y01	CAU-CAS	6.23	1.65	1.53
7	A	2229	Y01	CAK-CAI	-6.10	1.37	1.50
7	A	2229	Y01	CBH-CAZ	-5.44	1.42	1.52
7	A	2229	Y01	CAQ-CBG	-5.41	1.43	1.54
7	A	2229	Y01	CBB-CBE	5.31	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2229	Y01	CAE-CBI	-5.06	1.45	1.54
7	A	2229	Y01	CBI-CBE	4.86	1.63	1.55
7	A	2225	Y01	CAK-CAI	-4.51	1.41	1.50
7	A	2221	Y01	CAK-CAI	-4.51	1.41	1.50
7	A	2220	Y01	CAK-CAI	-4.49	1.41	1.50
7	A	2223	Y01	CAK-CAI	-4.46	1.41	1.50
7	A	2224	Y01	CAK-CAI	-4.46	1.41	1.50
7	A	2219	Y01	CAK-CAI	-4.45	1.41	1.50
7	A	2227	Y01	CAK-CAI	-4.42	1.41	1.50
7	A	2218	Y01	CAK-CAI	-4.42	1.41	1.50
7	A	2222	Y01	CAK-CAI	-4.42	1.41	1.50
7	A	2230	Y01	CAK-CAI	-4.41	1.41	1.50
7	A	2226	Y01	CAK-CAI	-4.40	1.41	1.50
7	A	2228	Y01	CAK-CAI	-4.39	1.41	1.50
7	A	2229	Y01	CAV-CAZ	-4.39	1.42	1.51
7	A	2229	Y01	CAU-CBI	4.28	1.61	1.54
7	A	2229	Y01	CBH-CBF	4.22	1.62	1.56
6	A	2217	6OU	O18-C16	4.01	1.45	1.33
6	A	2212	6OU	O18-C16	4.00	1.45	1.33
6	A	2213	6OU	O18-C16	3.99	1.45	1.33
6	A	2216	6OU	O18-C16	3.98	1.44	1.33
6	A	2215	6OU	O18-C16	3.97	1.44	1.33
6	A	2214	6OU	O18-C16	3.95	1.44	1.33
6	A	2217	6OU	O30-C31	3.93	1.45	1.34
6	A	2216	6OU	O30-C31	3.90	1.45	1.34
6	A	2213	6OU	O30-C31	3.88	1.45	1.34
6	A	2212	6OU	O30-C31	3.88	1.45	1.34
6	A	2215	6OU	O30-C31	3.87	1.45	1.34
6	A	2214	6OU	O30-C31	3.86	1.45	1.34
7	A	2229	Y01	CAK-CBD	-3.46	1.47	1.53
7	A	2229	Y01	CBI-CBG	-3.06	1.49	1.55
7	A	2229	Y01	CAP-CBE	-2.90	1.48	1.54
7	A	2229	Y01	CAD-CBH	-2.89	1.49	1.54
5	A	2211	XHO	C10-N09	2.83	1.41	1.35
6	A	2214	6OU	O30-C20	-2.81	1.40	1.46
7	A	2228	Y01	CAI-CAZ	2.79	1.38	1.33
7	A	2222	Y01	CAI-CAZ	2.79	1.38	1.33
7	A	2227	Y01	CAI-CAZ	2.78	1.38	1.33
7	A	2219	Y01	CAI-CAZ	2.77	1.38	1.33
7	A	2221	Y01	CAI-CAZ	2.76	1.38	1.33
7	A	2218	Y01	CAI-CAZ	2.76	1.38	1.33
7	A	2224	Y01	CAI-CAZ	2.76	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2220	Y01	CAI-CAZ	2.75	1.38	1.33
7	A	2230	Y01	CAI-CAZ	2.73	1.38	1.33
7	A	2226	Y01	CAI-CAZ	2.72	1.38	1.33
7	A	2223	Y01	CAI-CAZ	2.72	1.38	1.33
6	A	2215	6OU	O30-C20	-2.71	1.40	1.46
6	A	2217	6OU	P23-O26	2.70	1.67	1.58
7	A	2225	Y01	CAI-CAZ	2.69	1.38	1.33
6	A	2216	6OU	O30-C20	-2.66	1.40	1.46
6	A	2213	6OU	O30-C20	-2.65	1.40	1.46
6	A	2212	6OU	O30-C20	-2.63	1.40	1.46
7	A	2225	Y01	CBH-CAZ	-2.61	1.47	1.52
6	A	2217	6OU	C15-C16	2.58	1.58	1.50
6	A	2217	6OU	O30-C20	-2.55	1.40	1.46
7	A	2227	Y01	CBH-CAZ	-2.53	1.48	1.52
6	A	2213	6OU	C15-C16	2.52	1.58	1.50
7	A	2229	Y01	CAT-CAR	-2.51	1.48	1.53
6	A	2214	6OU	C15-C16	2.49	1.57	1.50
6	A	2213	6OU	C33-C31	2.49	1.57	1.50
7	A	2219	Y01	CBH-CAZ	-2.48	1.48	1.52
7	A	2230	Y01	CBH-CAZ	-2.47	1.48	1.52
6	A	2215	6OU	C15-C16	2.47	1.57	1.50
6	A	2212	6OU	C15-C16	2.47	1.57	1.50
6	A	2214	6OU	C33-C31	2.46	1.57	1.50
7	A	2229	Y01	CAJ-CAO	2.46	1.62	1.52
6	A	2212	6OU	C33-C31	2.46	1.57	1.50
6	A	2216	6OU	C33-C31	2.45	1.57	1.50
6	A	2216	6OU	C15-C16	2.44	1.57	1.50
7	A	2226	Y01	CBH-CAZ	-2.43	1.48	1.52
6	A	2215	6OU	C33-C31	2.42	1.57	1.50
6	A	2217	6OU	C33-C31	2.42	1.57	1.50
7	A	2229	Y01	CAI-CAZ	2.41	1.37	1.33
5	A	2211	XHO	C21-C20	2.33	1.59	1.51
7	A	2230	Y01	CAL-CAX	2.32	1.56	1.50
7	A	2228	Y01	CAL-CAX	2.27	1.55	1.50
6	A	2217	6OU	P23-O22	2.25	1.68	1.59
6	A	2215	6OU	P23-O22	2.22	1.68	1.59
6	A	2216	6OU	P23-O22	2.22	1.68	1.59
6	A	2213	6OU	P23-O22	2.21	1.68	1.59
6	A	2214	6OU	P23-O22	2.21	1.68	1.59
6	A	2212	6OU	P23-O22	2.20	1.68	1.59
7	A	2224	Y01	CBH-CAZ	-2.20	1.48	1.52
7	A	2227	Y01	CAL-CAX	2.19	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2223	Y01	CBH-CAZ	-2.18	1.48	1.52
5	A	2211	XHO	C19-N16	2.18	1.51	1.47
7	A	2222	Y01	CAL-CAX	2.18	1.55	1.50
7	A	2224	Y01	CAL-CAX	2.17	1.55	1.50
6	A	2215	6OU	P23-O26	2.16	1.67	1.59
7	A	2221	Y01	CBH-CAZ	-2.16	1.48	1.52
6	A	2212	6OU	P23-O26	2.15	1.67	1.59
6	A	2214	6OU	P23-O26	2.15	1.67	1.59
6	A	2213	6OU	P23-O26	2.12	1.67	1.59
7	A	2219	Y01	CAV-CAZ	-2.12	1.47	1.51
7	A	2221	Y01	CAL-CAX	2.12	1.55	1.50
6	A	2216	6OU	P23-O26	2.11	1.67	1.59
7	A	2222	Y01	CAQ-CBG	-2.09	1.50	1.54
7	A	2229	Y01	OAW-CAY	-2.08	1.28	1.34
7	A	2218	Y01	CBH-CAZ	-2.08	1.48	1.52
7	A	2220	Y01	CBH-CAZ	-2.06	1.48	1.52
7	A	2225	Y01	CBI-CBG	-2.03	1.51	1.55
7	A	2220	Y01	CAL-CAX	2.02	1.55	1.50
7	A	2221	Y01	CAV-CAZ	-2.01	1.47	1.51

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2226	Y01	CAV-CAZ-CBH	8.30	127.05	116.42
7	A	2227	Y01	CAV-CAZ-CBH	8.12	126.82	116.42
7	A	2229	Y01	OAW-CAY-CAM	7.98	128.75	111.48
7	A	2224	Y01	CAV-CAZ-CBH	7.95	126.60	116.42
7	A	2230	Y01	CAV-CAZ-CBH	7.94	126.59	116.42
7	A	2228	Y01	CAV-CAZ-CBH	7.94	126.58	116.42
7	A	2218	Y01	CAV-CAZ-CBH	7.91	126.54	116.42
7	A	2222	Y01	CAV-CAZ-CBH	7.76	126.36	116.42
7	A	2223	Y01	CAV-CAZ-CBH	7.73	126.32	116.42
7	A	2220	Y01	CAV-CAZ-CBH	7.64	126.21	116.42
7	A	2229	Y01	OAW-CAY-OAG	-7.61	105.91	123.70
7	A	2219	Y01	CAV-CAZ-CBH	7.45	125.97	116.42
7	A	2221	Y01	CAV-CAZ-CBH	7.42	125.93	116.42
7	A	2225	Y01	CAV-CAZ-CBH	7.25	125.71	116.42
7	A	2229	Y01	CAP-CBE-CBI	-7.24	95.32	103.84
7	A	2229	Y01	CAS-CBF-CBH	6.51	121.12	113.08
7	A	2229	Y01	CAS-CBF-CBD	-5.73	103.78	111.78
7	A	2229	Y01	CAT-CBH-CBF	5.69	116.27	108.74
7	A	2220	Y01	OAW-CAY-CAM	5.45	123.26	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2225	Y01	OAW-CAY-CAM	5.41	123.19	111.48
7	A	2222	Y01	OAW-CAY-CAM	5.41	123.17	111.48
7	A	2220	Y01	OAW-CAY-OAG	-5.33	111.24	123.70
7	A	2223	Y01	OAW-CAY-CAM	5.33	123.00	111.48
7	A	2224	Y01	OAW-CAY-OAG	-5.30	111.32	123.70
7	A	2219	Y01	OAW-CAY-OAG	-5.29	111.33	123.70
7	A	2224	Y01	OAW-CAY-CAM	5.29	122.92	111.48
7	A	2227	Y01	OAW-CAY-CAM	5.28	122.91	111.48
7	A	2219	Y01	OAW-CAY-CAM	5.28	122.90	111.48
7	A	2223	Y01	OAW-CAY-OAG	-5.26	111.41	123.70
7	A	2227	Y01	CAV-CAZ-CAI	-5.25	113.46	120.57
7	A	2230	Y01	OAW-CAY-CAM	5.24	122.82	111.48
7	A	2230	Y01	OAW-CAY-OAG	-5.22	111.50	123.70
7	A	2222	Y01	OAW-CAY-OAG	-5.18	111.59	123.70
7	A	2224	Y01	CAV-CAZ-CAI	-5.17	113.56	120.57
7	A	2227	Y01	OAW-CAY-OAG	-5.14	111.69	123.70
7	A	2229	Y01	CBI-CBE-CBB	5.12	127.40	119.50
7	A	2221	Y01	OAW-CAY-CAM	5.06	122.44	111.48
7	A	2225	Y01	OAW-CAY-OAG	-5.05	111.89	123.70
7	A	2223	Y01	CAV-CAZ-CAI	-5.05	113.72	120.57
7	A	2221	Y01	CAV-CAZ-CAI	-5.03	113.76	120.57
7	A	2228	Y01	CAV-CAZ-CAI	-5.01	113.78	120.57
7	A	2226	Y01	CAV-CAZ-CAI	-5.01	113.78	120.57
7	A	2220	Y01	CAV-CAZ-CAI	-4.99	113.81	120.57
7	A	2222	Y01	CAV-CAZ-CAI	-4.99	113.81	120.57
7	A	2218	Y01	CAV-CAZ-CAI	-4.96	113.84	120.57
7	A	2226	Y01	OAW-CAY-CAM	4.92	122.13	111.48
7	A	2219	Y01	CAV-CAZ-CAI	-4.90	113.92	120.57
7	A	2228	Y01	OAW-CAY-CAM	4.87	122.03	111.48
7	A	2226	Y01	OAW-CAY-OAG	-4.87	112.32	123.70
7	A	2221	Y01	OAW-CAY-OAG	-4.84	112.39	123.70
7	A	2230	Y01	CAV-CAZ-CAI	-4.79	114.08	120.57
6	A	2214	6OU	O30-C31-C33	4.59	121.41	111.48
7	A	2225	Y01	CAV-CAZ-CAI	-4.57	114.37	120.57
7	A	2229	Y01	CAU-CAS-CBF	4.55	120.86	113.14
7	A	2225	Y01	CAP-CBE-CBI	-4.48	98.57	103.84
7	A	2228	Y01	OAW-CAY-OAG	-4.34	113.56	123.70
6	A	2212	6OU	O30-C31-C33	4.08	120.31	111.48
7	A	2229	Y01	CAK-CBD-CBF	-4.03	105.06	109.72
6	A	2216	6OU	O30-C31-C33	4.03	120.20	111.48
6	A	2213	6OU	O30-C31-C33	4.03	120.20	111.48
6	A	2216	6OU	C42-C41-C40	3.89	153.97	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2213	6OU	C42-C41-C40	3.87	153.84	124.83
6	A	2215	6OU	O30-C31-C33	3.82	119.75	111.48
7	A	2229	Y01	CBF-CBH-CAZ	3.81	115.22	109.65
6	A	2214	6OU	C42-C41-C40	3.78	153.19	124.83
6	A	2217	6OU	O30-C31-C33	3.76	119.61	111.48
7	A	2228	Y01	OAW-CBC-CAR	3.63	116.95	108.37
7	A	2229	Y01	CAQ-CBG-CBI	-3.63	99.58	103.84
7	A	2229	Y01	CAC-CBB-CBE	3.62	118.32	112.88
5	A	2211	XHO	C10-C12-N13	-3.60	105.05	113.41
7	A	2229	Y01	CAS-CAU-CBI	3.58	118.77	112.74
7	A	2227	Y01	OAW-CBC-CAV	-3.56	100.70	108.04
3	A	2202	NAG	C1-O5-C5	3.55	116.94	112.19
7	A	2229	Y01	CAU-CBI-CBG	-3.52	101.97	107.25
7	A	2229	Y01	CAT-CBH-CAZ	-3.48	102.74	108.74
6	A	2212	6OU	C42-C41-C40	3.39	152.91	126.43
7	A	2229	Y01	CAD-CBH-CBF	-3.26	108.01	111.66
5	A	2211	XHO	O29-C28-C23	3.21	119.76	115.40
5	A	2211	XHO	C12-N13-C14	-3.20	106.17	111.14
7	A	2221	Y01	CAO-CBB-CBE	-3.18	107.63	113.52
7	A	2230	Y01	OAW-CBC-CAR	3.17	115.87	108.37
7	A	2228	Y01	CAP-CBE-CBI	-3.14	100.14	103.84
7	A	2229	Y01	CBH-CAZ-CAI	-3.12	118.37	122.93
7	A	2226	Y01	CAP-CBE-CBI	-3.12	100.17	103.84
7	A	2227	Y01	CAR-CBC-CAV	3.10	115.29	110.97
7	A	2219	Y01	OAW-CBC-CAV	-3.04	101.77	108.04
6	A	2214	6OU	O18-C16-C15	3.04	121.10	111.83
7	A	2224	Y01	OAW-CBC-CAV	-3.01	101.84	108.04
7	A	2218	Y01	OAW-CBC-CAV	-2.99	102.97	109.71
6	A	2216	6OU	O18-C16-C15	2.99	120.96	111.83
7	A	2222	Y01	CBH-CBF-CBD	-2.99	108.34	112.71
7	A	2229	Y01	CAD-CBH-CAT	-2.94	104.95	109.43
7	A	2222	Y01	OAW-CBC-CAR	2.93	115.30	108.37
6	A	2213	6OU	O18-C16-C15	2.93	120.77	111.83
7	A	2225	Y01	CAT-CBH-CAZ	-2.84	103.85	108.74
7	A	2229	Y01	CAC-CBB-CAO	-2.82	105.97	110.34
3	A	2202	NAG	C2-N2-C7	2.80	126.66	122.90
7	A	2222	Y01	CAU-CBI-CBG	-2.79	103.07	107.25
7	A	2223	Y01	OAW-CBC-CAV	-2.78	102.32	108.04
7	A	2220	Y01	OAW-CBC-CAV	-2.76	102.35	108.04
6	A	2215	6OU	O18-C16-C15	2.76	120.24	111.83
7	A	2230	Y01	CBF-CBD-CBG	2.72	112.63	109.09
7	A	2221	Y01	OAW-CBC-CAV	-2.70	102.47	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2225	Y01	CBF-CBH-CAZ	2.67	113.56	109.65
5	A	2211	XHO	C12-N13-C18	-2.67	107.00	111.14
3	A	2201	NAG	C2-N2-C7	2.66	126.47	122.90
7	A	2219	Y01	CBH-CBF-CBD	-2.66	108.83	112.71
3	A	2208	NAG	C2-N2-C7	2.63	126.42	122.90
7	A	2226	Y01	CAS-CBF-CBD	-2.62	108.12	111.78
7	A	2226	Y01	OAW-CBC-CAV	-2.62	102.65	108.04
7	A	2229	Y01	CAE-CBI-CAU	2.61	114.46	110.61
6	A	2217	6OU	O18-C16-C15	2.59	119.74	111.83
7	A	2223	Y01	OAW-CBC-CAR	2.58	114.47	108.37
7	A	2226	Y01	CBH-CAZ-CAI	-2.58	119.17	122.93
7	A	2228	Y01	CBH-CBF-CBD	-2.54	109.00	112.71
7	A	2221	Y01	CBF-CBD-CBG	2.53	112.40	109.09
7	A	2225	Y01	OAW-CBC-CAV	-2.52	102.84	108.04
7	A	2221	Y01	CBH-CBF-CBD	-2.52	109.03	112.71
7	A	2224	Y01	OAW-CBC-CAR	2.48	114.22	108.37
7	A	2230	Y01	CBH-CAZ-CAI	-2.47	119.33	122.93
7	A	2224	Y01	CAP-CBE-CBB	-2.45	108.47	112.18
6	A	2212	6OU	O18-C16-C15	2.45	119.30	111.83
7	A	2220	Y01	OAW-CBC-CAR	2.44	114.15	108.37
7	A	2227	Y01	CAP-CBE-CBI	-2.43	100.98	103.84
7	A	2226	Y01	CBG-CBI-CBE	-2.43	97.31	100.10
7	A	2219	Y01	OAW-CBC-CAR	2.42	114.10	108.37
7	A	2223	Y01	CAS-CBF-CBD	-2.41	108.42	111.78
7	A	2222	Y01	OAW-CBC-CAV	-2.41	103.08	108.04
7	A	2228	Y01	CBF-CBD-CBG	2.40	112.22	109.09
7	A	2227	Y01	OAW-CBC-CAR	2.40	114.03	108.37
6	A	2212	6OU	C39-C40-C41	-2.39	112.40	130.48
7	A	2219	Y01	CAP-CBE-CBB	-2.38	108.57	112.18
7	A	2226	Y01	CAP-CBE-CBB	-2.38	108.58	112.18
7	A	2222	Y01	CBG-CBI-CBE	2.38	102.83	100.10
7	A	2230	Y01	CBH-CBF-CBD	-2.37	109.25	112.71
7	A	2219	Y01	CBF-CBD-CBG	2.35	112.16	109.09
7	A	2226	Y01	CBD-CAK-CAI	2.34	116.00	112.76
7	A	2225	Y01	CAS-CBF-CBD	-2.30	108.58	111.78
7	A	2222	Y01	CAP-CAQ-CBG	-2.27	100.70	105.14
7	A	2218	Y01	CBH-CAZ-CAI	-2.27	119.61	122.93
7	A	2227	Y01	CAT-CBH-CAZ	-2.27	104.83	108.74
7	A	2228	Y01	CBH-CAZ-CAI	-2.25	119.64	122.93
7	A	2230	Y01	CAP-CBE-CBI	-2.24	101.21	103.84
7	A	2227	Y01	CBF-CBD-CBG	2.23	112.00	109.09
7	A	2225	Y01	OAW-CBC-CAR	2.22	113.62	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2221	Y01	CAP-CBE-CBI	-2.21	102.31	104.30
7	A	2229	Y01	CBF-CBD-CBG	2.21	111.98	109.09
7	A	2222	Y01	CAP-CBE-CBB	-2.20	108.85	112.18
5	A	2211	XHO	O22-C21-C20	2.20	111.61	107.64
7	A	2227	Y01	CBH-CAZ-CAI	-2.20	119.72	122.93
7	A	2219	Y01	OAF-CAX-CAL	-2.19	116.14	123.09
7	A	2224	Y01	OAF-CAX-CAL	-2.19	116.16	123.09
7	A	2218	Y01	CAP-CBE-CBI	-2.18	101.27	103.84
7	A	2220	Y01	OAF-CAX-CAL	-2.18	116.17	123.09
7	A	2226	Y01	OAF-CAX-CAL	-2.18	116.19	123.09
7	A	2222	Y01	OAF-CAX-CAL	-2.17	116.22	123.09
7	A	2227	Y01	OAF-CAX-CAL	-2.17	116.22	123.09
7	A	2221	Y01	OAF-CAX-CAL	-2.17	116.22	123.09
7	A	2229	Y01	CAQ-CAP-CBE	2.17	109.38	105.14
7	A	2223	Y01	OAF-CAX-CAL	-2.17	116.22	123.09
7	A	2223	Y01	CAP-CBE-CBB	-2.16	108.90	112.18
7	A	2221	Y01	OAW-CBC-CAR	2.16	113.48	108.37
7	A	2222	Y01	CBI-CBG-CBD	-2.16	111.34	114.41
7	A	2225	Y01	OAF-CAX-CAL	-2.13	116.33	123.09
7	A	2227	Y01	CBH-CBF-CBD	-2.13	109.60	112.71
7	A	2228	Y01	OAF-CAX-CAL	-2.12	116.35	123.09
7	A	2222	Y01	CBH-CAZ-CAI	-2.12	119.83	122.93
7	A	2224	Y01	CBH-CAZ-CAI	-2.11	119.84	122.93
7	A	2221	Y01	CAR-CBC-CAV	2.11	113.91	110.97
7	A	2218	Y01	CAS-CBF-CBD	-2.11	108.84	111.78
7	A	2221	Y01	CAT-CBH-CAZ	-2.09	105.15	108.74
7	A	2230	Y01	OAF-CAX-CAL	-2.08	116.49	123.09
7	A	2229	Y01	CAV-CAZ-CBH	2.08	119.08	116.42
7	A	2222	Y01	CAU-CAS-CBF	2.06	116.64	113.14
7	A	2225	Y01	CBH-CAZ-CAI	-2.06	119.92	122.93
5	A	2211	XHO	O22-C23-C28	2.06	120.00	115.75
7	A	2230	Y01	CAP-CBE-CBB	-2.06	109.07	112.18
7	A	2223	Y01	CBH-CAZ-CAI	-2.04	119.95	122.93
5	A	2211	XHO	C19-C20-C21	-2.03	107.06	111.59
6	A	2213	6OU	C20-O30-C31	-2.03	112.94	117.80
6	A	2215	6OU	C39-C40-C41	-2.02	111.93	126.65
7	A	2220	Y01	CBH-CAZ-CAI	-2.02	119.98	122.93
7	A	2229	Y01	OAW-CBC-CAR	2.01	113.11	108.37

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2201	NAG	C1-C2-N2-C7
3	A	2202	NAG	C1-C2-N2-C7
3	A	2208	NAG	C1-C2-N2-C7
5	A	2211	XHO	N16-C19-C20-C21
5	A	2211	XHO	N16-C19-C20-O31
6	A	2212	6OU	C27-O26-P23-O24
6	A	2212	6OU	O26-C27-C28-N29
6	A	2213	6OU	C21-O22-P23-O25
6	A	2213	6OU	C21-O22-P23-O26
6	A	2213	6OU	O26-C27-C28-N29
6	A	2213	6OU	C33-C31-O30-C20
6	A	2214	6OU	O26-C27-C28-N29
6	A	2214	6OU	O32-C31-O30-C20
6	A	2215	6OU	C21-O22-P23-O25
6	A	2215	6OU	C21-O22-P23-O26
6	A	2215	6OU	C27-O26-P23-O22
6	A	2215	6OU	C27-O26-P23-O25
6	A	2215	6OU	O26-C27-C28-N29
6	A	2216	6OU	C27-O26-P23-O22
6	A	2216	6OU	C27-O26-P23-O24
6	A	2216	6OU	O26-C27-C28-N29
6	A	2217	6OU	C27-O26-P23-O25
7	A	2219	Y01	CAM-CAY-OAW-CBC
7	A	2220	Y01	CAM-CAY-OAW-CBC
7	A	2222	Y01	CAR-CBC-OAW-CAY
7	A	2223	Y01	CAR-CBC-OAW-CAY
7	A	2223	Y01	CAM-CAY-OAW-CBC
7	A	2224	Y01	OAG-CAY-OAW-CBC
7	A	2224	Y01	CAM-CAY-OAW-CBC
7	A	2227	Y01	CAM-CAY-OAW-CBC
7	A	2229	Y01	CAM-CAY-OAW-CBC
7	A	2230	Y01	CAM-CAY-OAW-CBC
6	A	2213	6OU	O17-C16-O18-C19
7	A	2219	Y01	CAR-CBC-OAW-CAY
7	A	2224	Y01	CAR-CBC-OAW-CAY
7	A	2227	Y01	CAR-CBC-OAW-CAY
7	A	2228	Y01	CAR-CBC-OAW-CAY
7	A	2229	Y01	CAR-CBC-OAW-CAY
7	A	2230	Y01	CAR-CBC-OAW-CAY
6	A	2213	6OU	C15-C16-O18-C19
6	A	2214	6OU	O17-C16-O18-C19
6	A	2217	6OU	O17-C16-O18-C19
7	A	2226	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
6	A	2213	6OU	O32-C31-O30-C20
7	A	2220	Y01	OAG-CAY-OAW-CBC
7	A	2223	Y01	OAG-CAY-OAW-CBC
7	A	2227	Y01	OAG-CAY-OAW-CBC
7	A	2229	Y01	OAG-CAY-OAW-CBC
7	A	2230	Y01	OAG-CAY-OAW-CBC
6	A	2212	6OU	C15-C16-O18-C19
6	A	2214	6OU	C15-C16-O18-C19
6	A	2214	6OU	C33-C31-O30-C20
7	A	2229	Y01	CAO-CBB-CBE-CBI
7	A	2227	Y01	CAX-CAL-CAM-CAY
3	A	2208	NAG	O5-C5-C6-O6
6	A	2217	6OU	C15-C16-O18-C19
6	A	2212	6OU	O17-C16-O18-C19
7	A	2219	Y01	OAG-CAY-OAW-CBC
6	A	2212	6OU	C33-C31-O30-C20
7	A	2222	Y01	CAM-CAY-OAW-CBC
7	A	2226	Y01	CAC-CBB-CBE-CBI
7	A	2229	Y01	CAC-CBB-CBE-CBI
6	A	2212	6OU	O32-C31-O30-C20
3	A	2210	NAG	O5-C5-C6-O6
3	A	2208	NAG	C4-C5-C6-O6
6	A	2215	6OU	C15-C16-O18-C19
3	A	2209	NAG	O5-C5-C6-O6
6	A	2215	6OU	O17-C16-O18-C19
7	A	2222	Y01	OAG-CAY-OAW-CBC
7	A	2226	Y01	CAC-CBB-CBE-CAP
3	A	2201	NAG	O5-C5-C6-O6
6	A	2216	6OU	C33-C31-O30-C20
3	A	2201	NAG	C8-C7-N2-C2
3	A	2201	NAG	O7-C7-N2-C2
3	A	2202	NAG	C8-C7-N2-C2
3	A	2202	NAG	O7-C7-N2-C2
3	A	2208	NAG	C8-C7-N2-C2
3	A	2208	NAG	O7-C7-N2-C2
3	A	2209	NAG	C8-C7-N2-C2
3	A	2209	NAG	O7-C7-N2-C2
3	A	2210	NAG	C8-C7-N2-C2
3	A	2210	NAG	O7-C7-N2-C2
3	A	2205	NAG	O5-C5-C6-O6
3	A	2209	NAG	C4-C5-C6-O6
6	A	2215	6OU	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
7	A	2229	Y01	CAO-CAJ-CAN-CBA
7	A	2225	Y01	CAO-CAJ-CAN-CBA
7	A	2219	Y01	CAO-CAJ-CAN-CBA
4	A	2207	BMA	O5-C5-C6-O6
5	A	2211	XHO	C20-C19-N16-C15
6	A	2216	6OU	O32-C31-O30-C20
7	A	2229	Y01	CAN-CAJ-CAO-CBB
7	A	2226	Y01	CAN-CAJ-CAO-CBB
6	A	2217	6OU	C33-C31-O30-C20
6	A	2217	6OU	O32-C31-O30-C20
3	A	2210	NAG	C4-C5-C6-O6
7	A	2230	Y01	CAJ-CAN-CBA-CAB
6	A	2212	6OU	C10-C11-C12-C13
7	A	2218	Y01	CAJ-CAN-CBA-CAA
7	A	2227	Y01	CAO-CAJ-CAN-CBA
6	A	2215	6OU	C04-C05-C06-C07
6	A	2214	6OU	C06-C07-C08-C09
6	A	2216	6OU	C44-C45-C46-C47
7	A	2218	Y01	CAJ-CAN-CBA-CAB
7	A	2223	Y01	CAJ-CAN-CBA-CAB
7	A	2224	Y01	CAJ-CAN-CBA-CAB
7	A	2228	Y01	CAJ-CAN-CBA-CAA
6	A	2213	6OU	C13-C14-C15-C16
7	A	2230	Y01	CAJ-CAN-CBA-CAA
6	A	2214	6OU	C07-C08-C09-C10
7	A	2218	Y01	CAO-CAJ-CAN-CBA
6	A	2213	6OU	C43-C44-C45-C46
6	A	2215	6OU	C06-C07-C08-C09
6	A	2215	6OU	C10-C11-C12-C13
6	A	2214	6OU	C37-C38-C39-C40
6	A	2215	6OU	C33-C34-C35-C36
6	A	2217	6OU	C12-C13-C14-C15
6	A	2217	6OU	C04-C05-C06-C07
6	A	2214	6OU	C12-C13-C14-C15
6	A	2216	6OU	C37-C38-C39-C40
6	A	2213	6OU	C09-C10-C11-C12
6	A	2215	6OU	C36-C37-C38-C39
3	A	2202	NAG	O5-C5-C6-O6
6	A	2213	6OU	C37-C38-C39-C40
6	A	2216	6OU	C11-C12-C13-C14
7	A	2218	Y01	CAN-CAJ-CAO-CBB
5	A	2211	XHO	C20-C19-N16-C17

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Mol	Chain	Res	Type	Atoms
6	A	2213	6OU	C35-C36-C37-C38
6	A	2214	6OU	C02-C03-C04-C05
6	A	2213	6OU	C33-C34-C35-C36
6	A	2214	6OU	C44-C45-C46-C47
6	A	2216	6OU	C13-C14-C15-C16
7	A	2228	Y01	CAX-CAL-CAM-CAY
5	A	2211	XHO	C20-C21-O22-C23
6	A	2213	6OU	C41-C42-C43-C44
6	A	2215	6OU	C37-C38-C39-C40
7	A	2226	Y01	CAO-CBB-CBE-CBI
7	A	2223	Y01	CAJ-CAN-CBA-CAA
7	A	2229	Y01	CAC-CBB-CBE-CAP
7	A	2221	Y01	CAN-CAJ-CAO-CBB
6	A	2216	6OU	C15-C16-O18-C19
6	A	2216	6OU	C09-C10-C11-C12
7	A	2229	Y01	CAV-CBC-OAW-CAY
6	A	2214	6OU	O30-C20-C21-O22
6	A	2217	6OU	C36-C37-C38-C39
6	A	2213	6OU	C45-C46-C47-C48
6	A	2212	6OU	C37-C38-C39-C40
6	A	2215	6OU	C01-C02-C03-C04
6	A	2217	6OU	C37-C38-C39-C40
6	A	2214	6OU	C04-C05-C06-C07
6	A	2217	6OU	C07-C08-C09-C10
6	A	2215	6OU	C19-C20-C21-O22
7	A	2224	Y01	CAJ-CAO-CBB-CAC
7	A	2228	Y01	CAJ-CAN-CBA-CAB
6	A	2212	6OU	C33-C34-C35-C36
6	A	2216	6OU	O17-C16-O18-C19
5	A	2211	XHO	C24-C23-O22-C21
6	A	2217	6OU	O18-C19-C20-C21
6	A	2215	6OU	C02-C03-C04-C05
6	A	2217	6OU	C06-C07-C08-C09
7	A	2229	Y01	CAO-CBB-CBE-CAP
5	A	2211	XHO	N09-C10-C12-N13
6	A	2216	6OU	C12-C13-C14-C15
7	A	2224	Y01	CAJ-CAN-CBA-CAA
6	A	2217	6OU	O18-C19-C20-O30
6	A	2215	6OU	C12-C13-C14-C15
5	A	2211	XHO	O11-C10-C12-N13
7	A	2218	Y01	CAJ-CAO-CBB-CAC
6	A	2213	6OU	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
6	A	2215	6OU	C34-C35-C36-C37
6	A	2214	6OU	C41-C42-C43-C44
6	A	2215	6OU	O30-C20-C21-O22
6	A	2215	6OU	O18-C19-C20-C21
6	A	2215	6OU	O18-C19-C20-O30
7	A	2224	Y01	CAV-CBC-OAW-CAY
6	A	2216	6OU	C46-C47-C48-C49
6	A	2214	6OU	C19-C20-C21-O22
7	A	2228	Y01	CAC-CBB-CBE-CBI
6	A	2212	6OU	O18-C19-C20-O30
6	A	2216	6OU	O18-C19-C20-C21
7	A	2229	Y01	CAJ-CAO-CBB-CBE
6	A	2216	6OU	C36-C37-C38-C39
6	A	2213	6OU	C21-O22-P23-O24
6	A	2214	6OU	C27-O26-P23-O24
6	A	2215	6OU	C27-O26-P23-O24
6	A	2216	6OU	C27-O26-P23-O25
6	A	2216	6OU	C19-C20-O30-C31
6	A	2212	6OU	C38-C39-C40-C41
6	A	2212	6OU	O18-C19-C20-C21
3	A	2201	NAG	C4-C5-C6-O6
6	A	2214	6OU	C40-C41-C42-C43
6	A	2214	6OU	C10-C11-C12-C13
7	A	2228	Y01	CAO-CBB-CBE-CBI
7	A	2223	Y01	CAO-CAJ-CAN-CBA
6	A	2214	6OU	C43-C44-C45-C46
6	A	2216	6OU	O30-C20-C21-O22
7	A	2229	Y01	CAJ-CAN-CBA-CAB
6	A	2217	6OU	C34-C35-C36-C37
6	A	2212	6OU	C35-C36-C37-C38
7	A	2228	Y01	CAM-CAL-CAX-OAF
6	A	2217	6OU	C19-C20-O30-C31
6	A	2217	6OU	C21-C20-O30-C31
5	A	2211	XHO	C28-C23-O22-C21
6	A	2212	6OU	C34-C35-C36-C37
7	A	2219	Y01	CAM-CAL-CAX-OAF
7	A	2221	Y01	CAM-CAL-CAX-OAH
7	A	2220	Y01	CAM-CAL-CAX-OAF
7	A	2227	Y01	CAM-CAL-CAX-OAF
7	A	2228	Y01	CAM-CAL-CAX-OAH
7	A	2229	Y01	CAM-CAL-CAX-OAF
7	A	2221	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
7	A	2224	Y01	CAM-CAL-CAX-OAH
7	A	2225	Y01	CAJ-CAO-CBB-CAC
7	A	2223	Y01	CAO-CBB-CBE-CAP
6	A	2216	6OU	O18-C19-C20-O30
7	A	2226	Y01	CAM-CAL-CAX-OAF
7	A	2222	Y01	CAM-CAL-CAX-OAH
7	A	2219	Y01	CAV-CBC-OAW-CAY
7	A	2225	Y01	CAR-CBC-OAW-CAY
6	A	2216	6OU	C08-C09-C10-C11
7	A	2224	Y01	CAM-CAL-CAX-OAF
7	A	2229	Y01	CAM-CAL-CAX-OAH
6	A	2216	6OU	C45-C46-C47-C48
7	A	2222	Y01	CAM-CAL-CAX-OAF
6	A	2216	6OU	C33-C34-C35-C36
7	A	2219	Y01	CAM-CAL-CAX-OAH
7	A	2223	Y01	CAM-CAL-CAX-OAF
7	A	2226	Y01	CAM-CAL-CAX-OAH
7	A	2220	Y01	CAL-CAM-CAY-OAW
6	A	2216	6OU	C40-C41-C42-C43
7	A	2220	Y01	CAM-CAL-CAX-OAH
6	A	2215	6OU	C05-C06-C07-C08
6	A	2214	6OU	C46-C47-C48-C49
7	A	2227	Y01	CAM-CAL-CAX-OAH
6	A	2216	6OU	C38-C39-C40-C41
6	A	2213	6OU	C20-C21-O22-P23
7	A	2223	Y01	CAM-CAL-CAX-OAH
6	A	2217	6OU	C35-C36-C37-C38
6	A	2213	6OU	C02-C03-C04-C05
7	A	2220	Y01	CAX-CAL-CAM-CAY
7	A	2226	Y01	CAL-CAM-CAY-OAW
6	A	2217	6OU	C14-C15-C16-O18
7	A	2227	Y01	CAL-CAM-CAY-OAW
7	A	2224	Y01	CAL-CAM-CAY-OAW
6	A	2213	6OU	C03-C04-C05-C06
7	A	2225	Y01	CAJ-CAN-CBA-CAB
6	A	2215	6OU	C21-C20-O30-C31
7	A	2225	Y01	CAJ-CAN-CBA-CAA
6	A	2217	6OU	C14-C15-C16-O17
7	A	2227	Y01	CAL-CAM-CAY-OAG
7	A	2226	Y01	CAL-CAM-CAY-OAG
6	A	2215	6OU	C09-C10-C11-C12
6	A	2214	6OU	C20-C21-O22-P23

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Mol	Chain	Res	Type	Atoms
6	A	2213	6OU	C14-C15-C16-O18

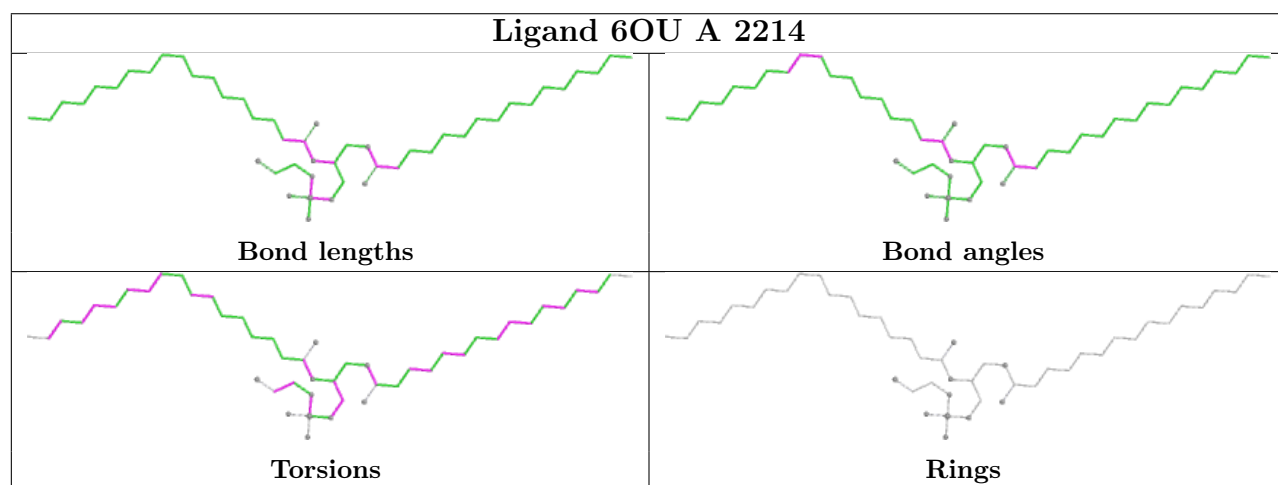
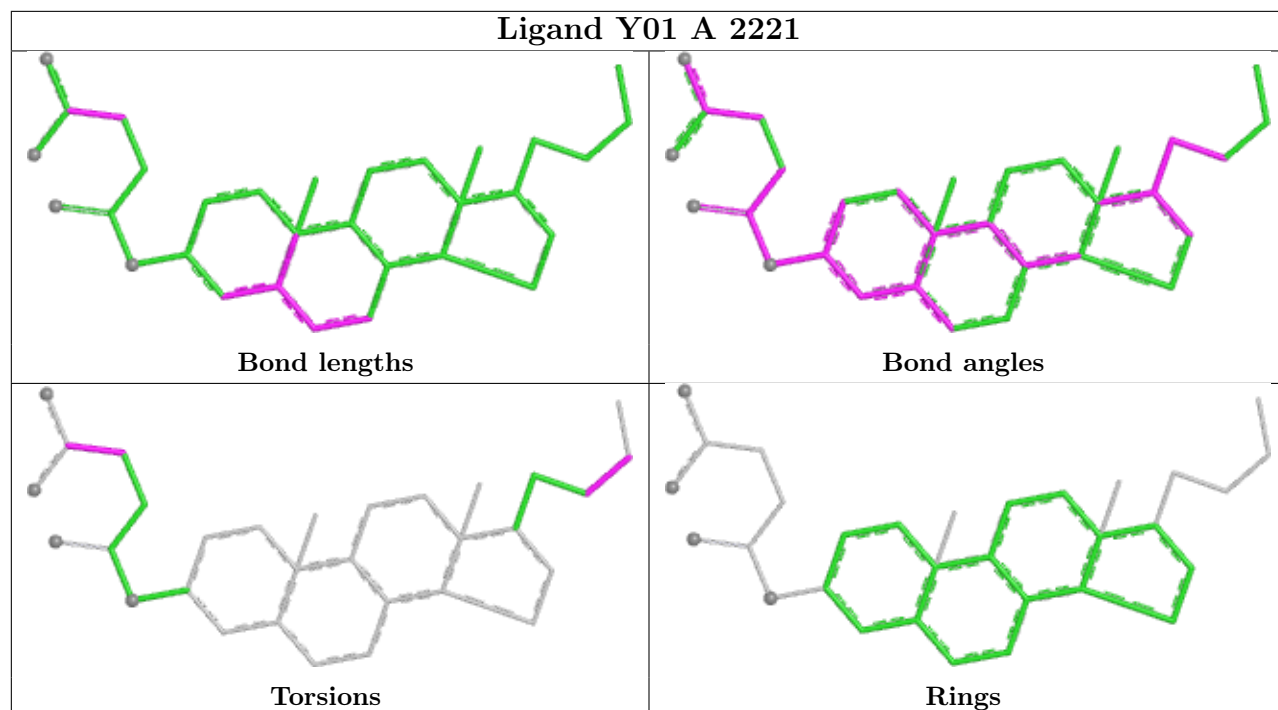
All (1) ring outliers are listed below:

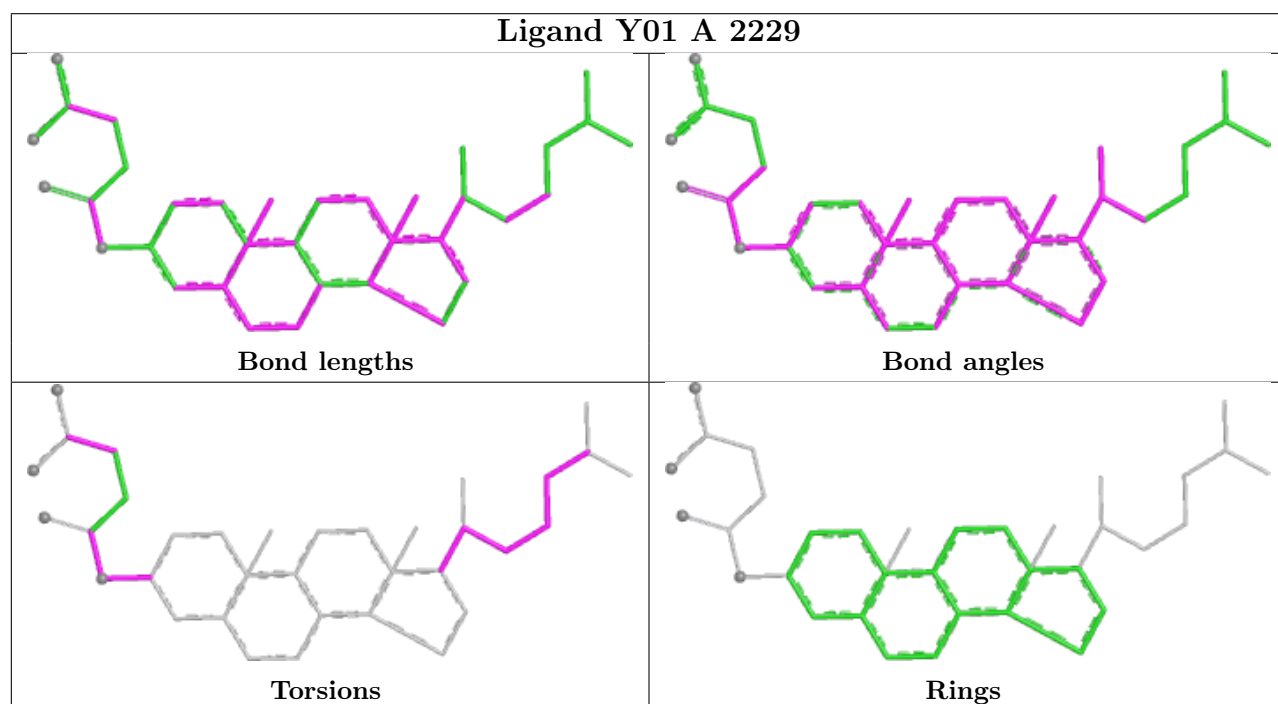
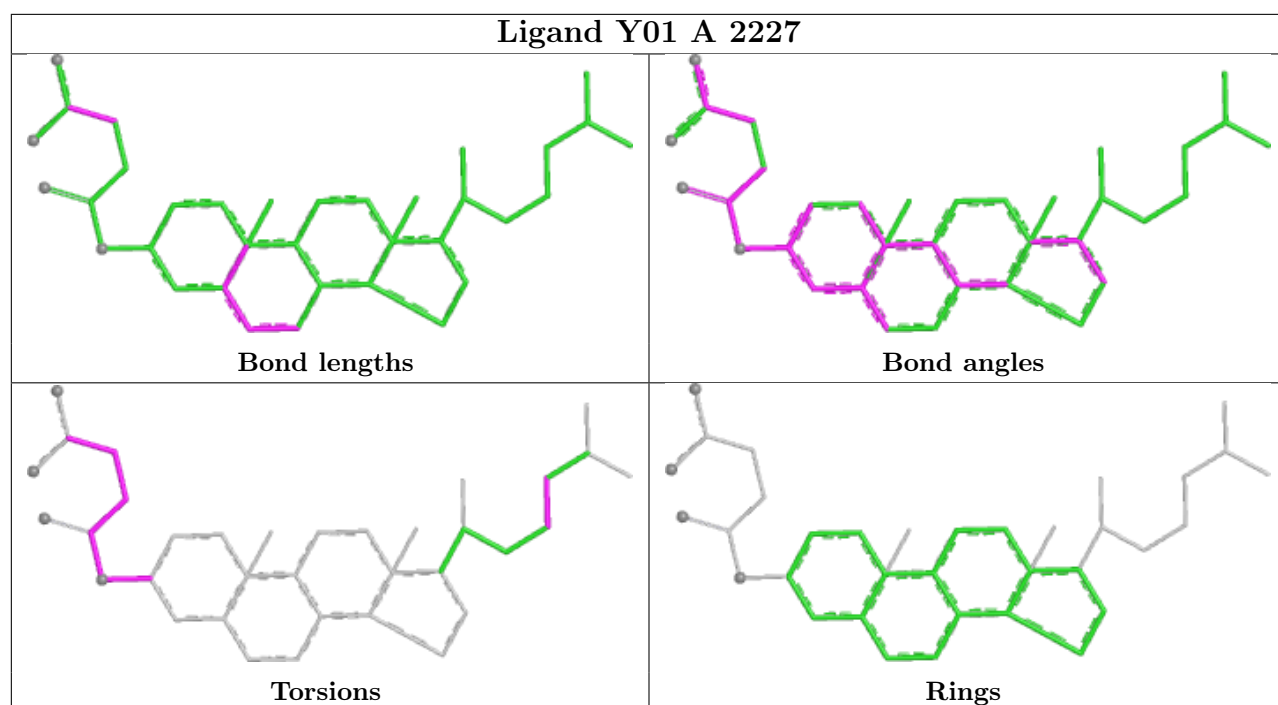
Mol	Chain	Res	Type	Atoms
4	A	2207	BMA	C1-C2-C3-C4-C5-O5

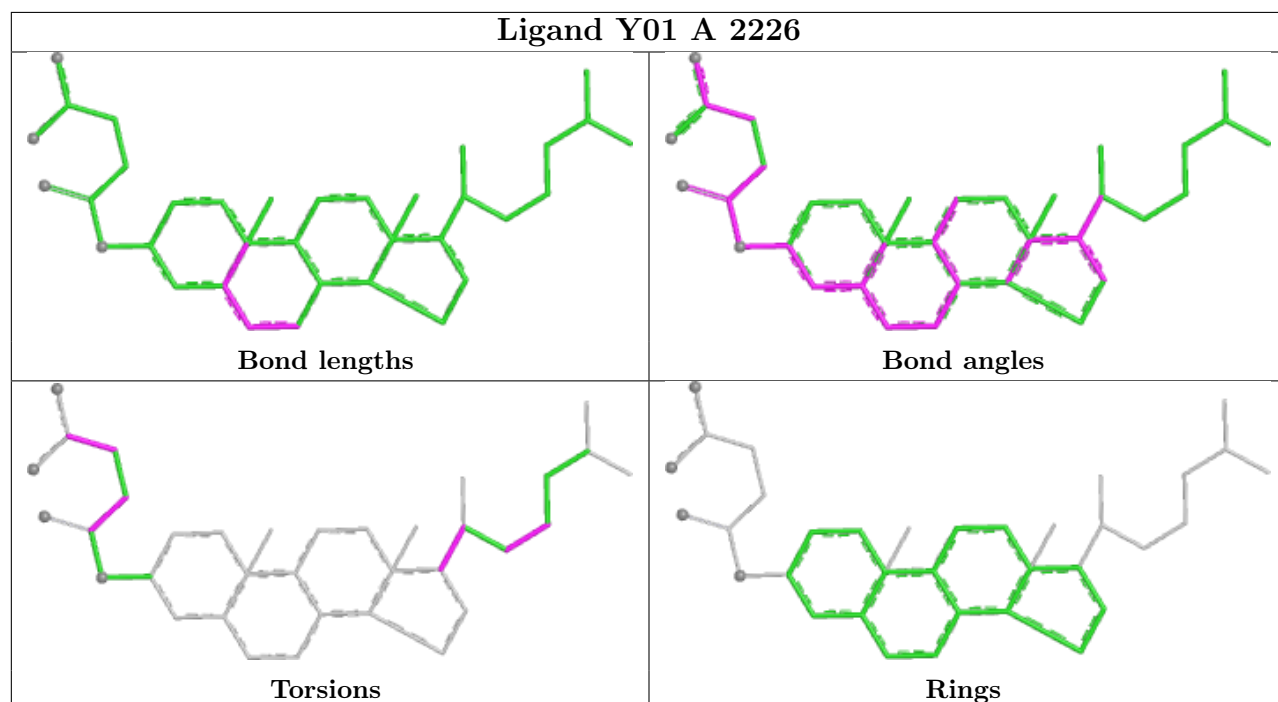
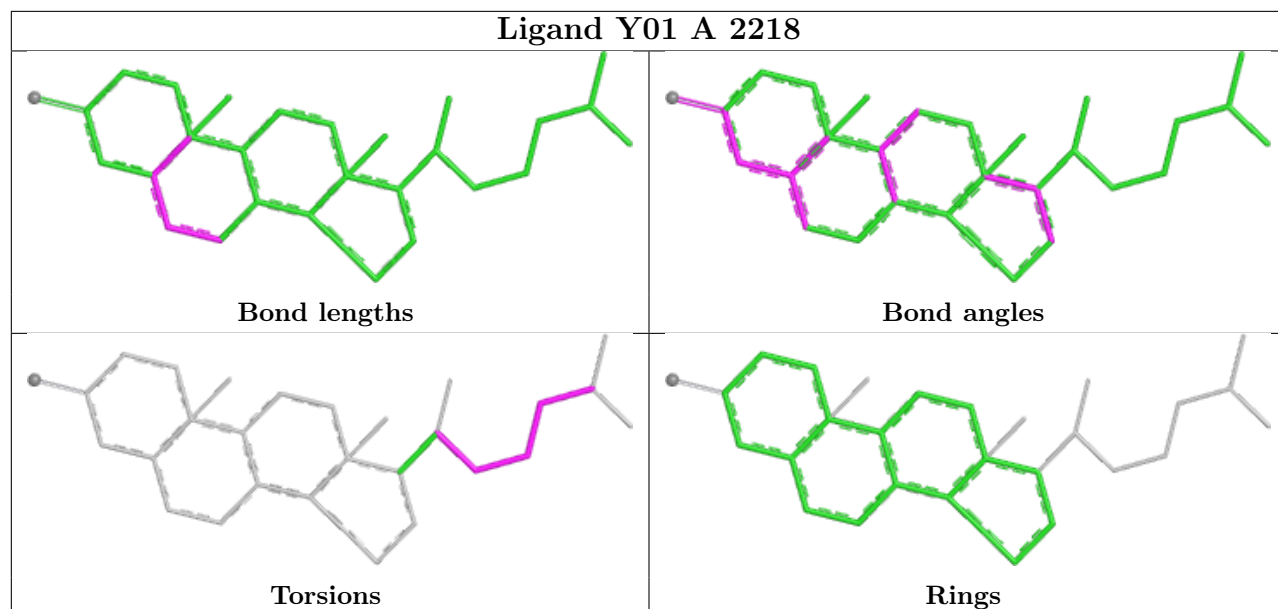
18 monomers are involved in 39 short contacts:

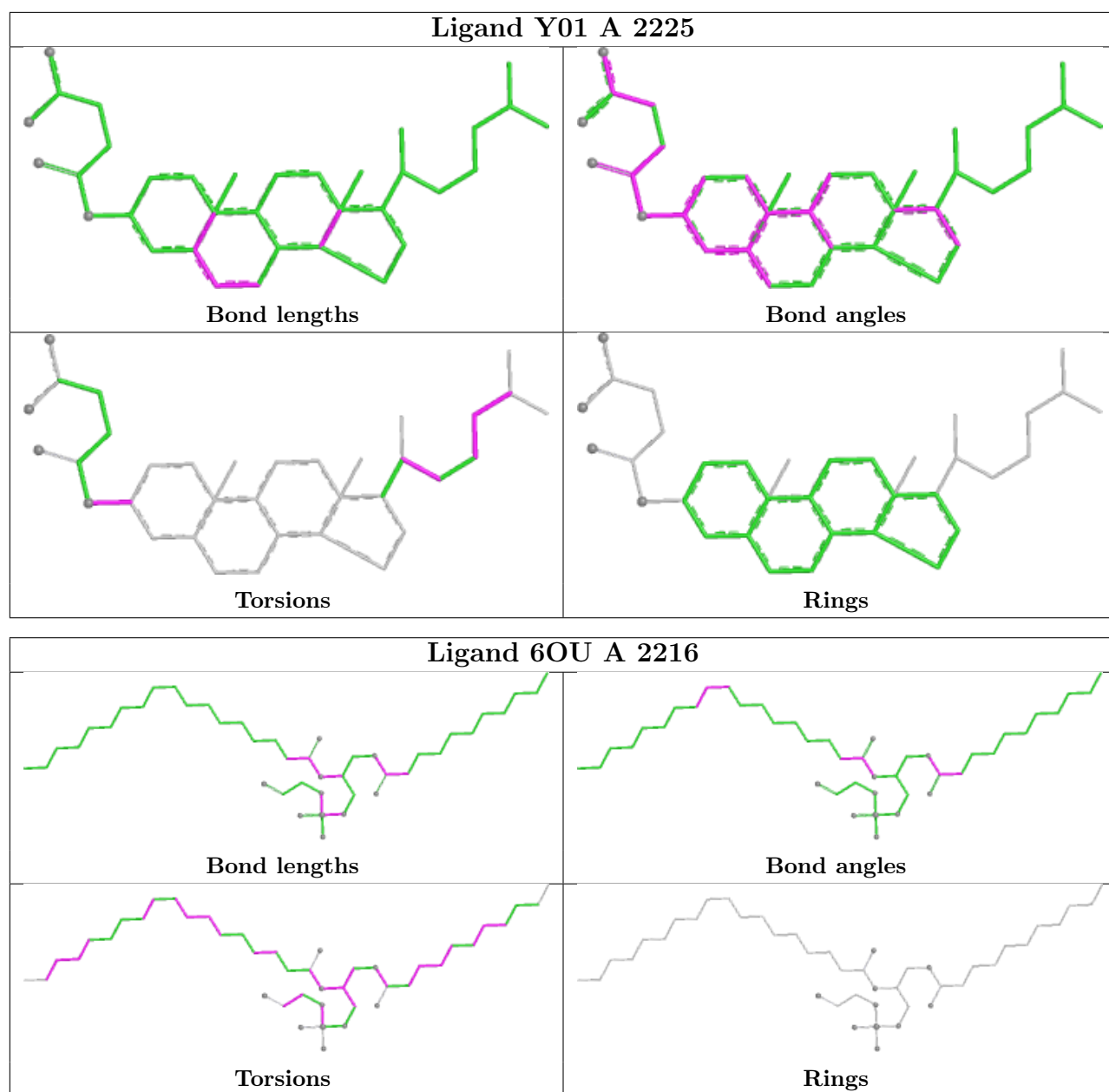
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2221	Y01	2	0
6	A	2214	6OU	1	0
7	A	2218	Y01	3	0
7	A	2226	Y01	2	0
7	A	2225	Y01	7	0
6	A	2216	6OU	1	0
3	A	2202	NAG	4	0
7	A	2223	Y01	1	0
5	A	2211	XHO	1	0
7	A	2219	Y01	3	0
4	A	2204	BMA	1	0
3	A	2201	NAG	3	0
4	A	2206	BMA	1	0
3	A	2208	NAG	5	0
4	A	2207	BMA	1	0
7	A	2222	Y01	3	0
7	A	2228	Y01	1	0
7	A	2224	Y01	1	0

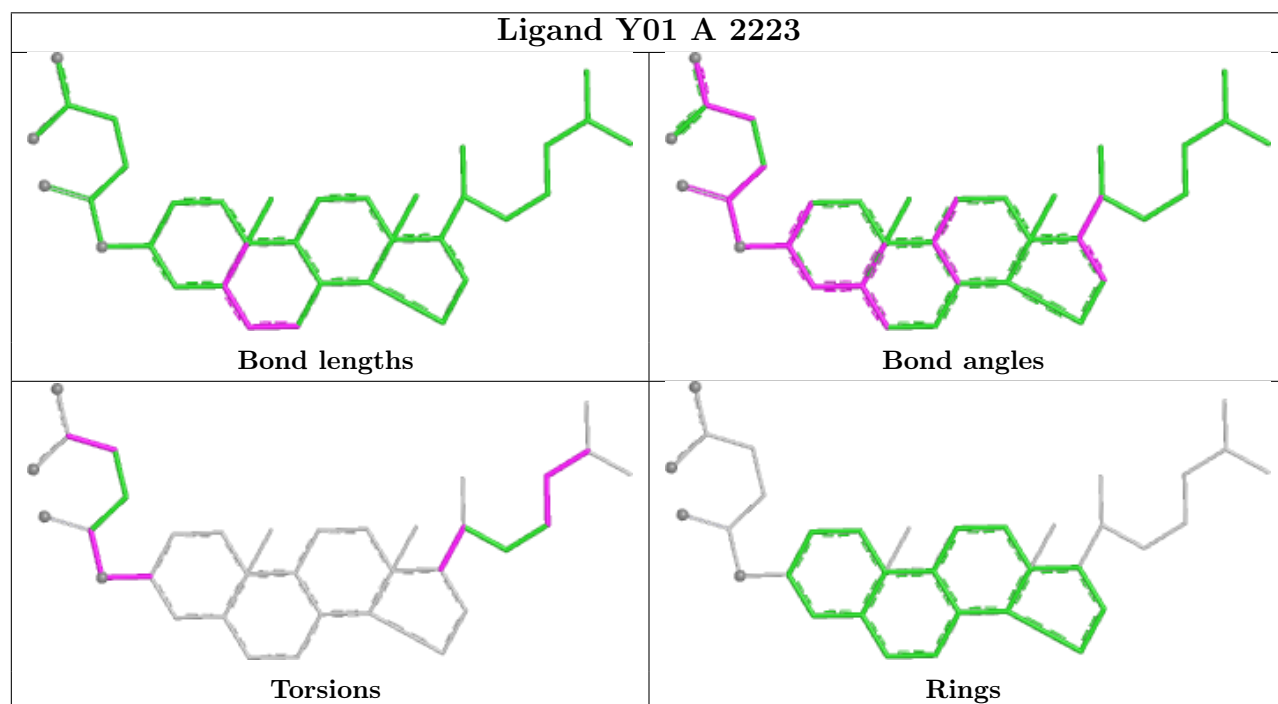
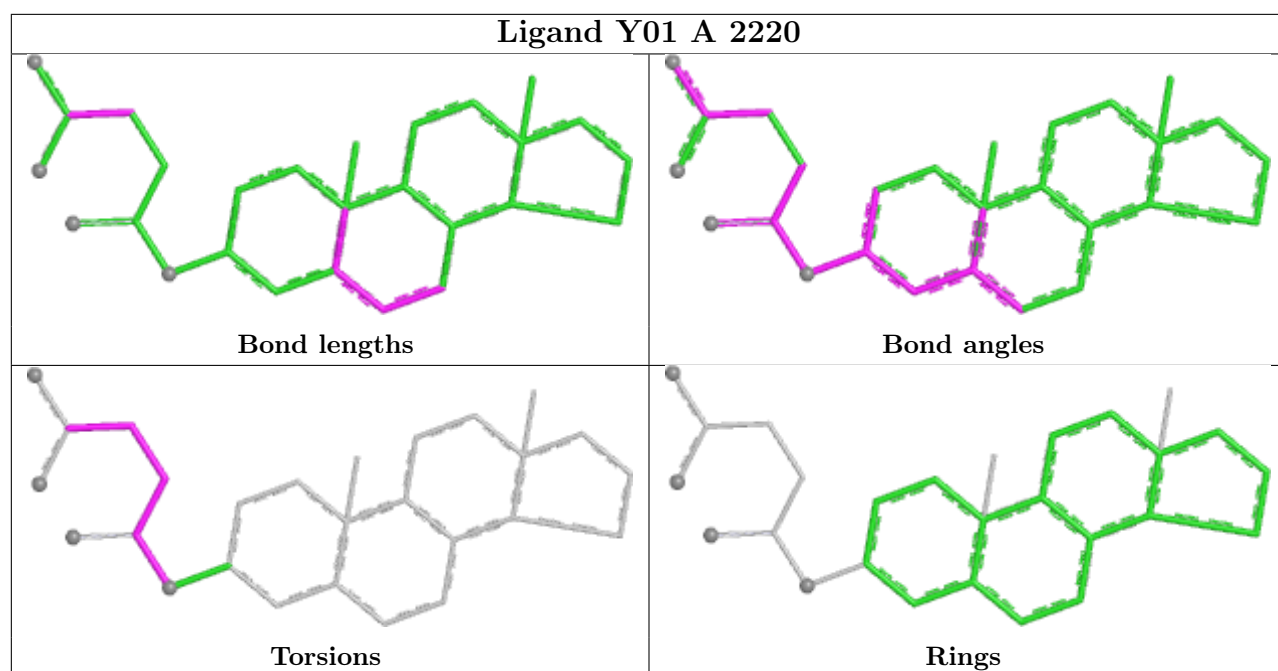
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

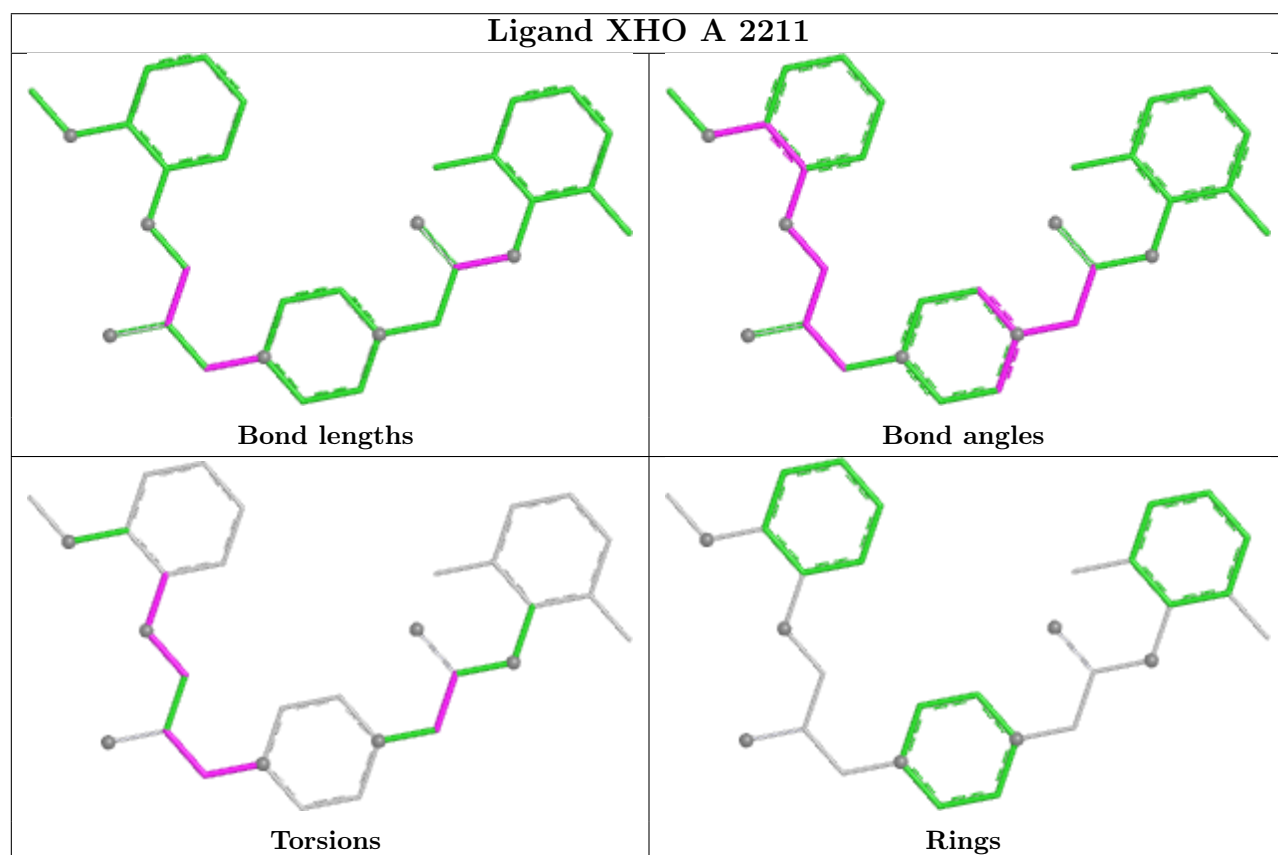
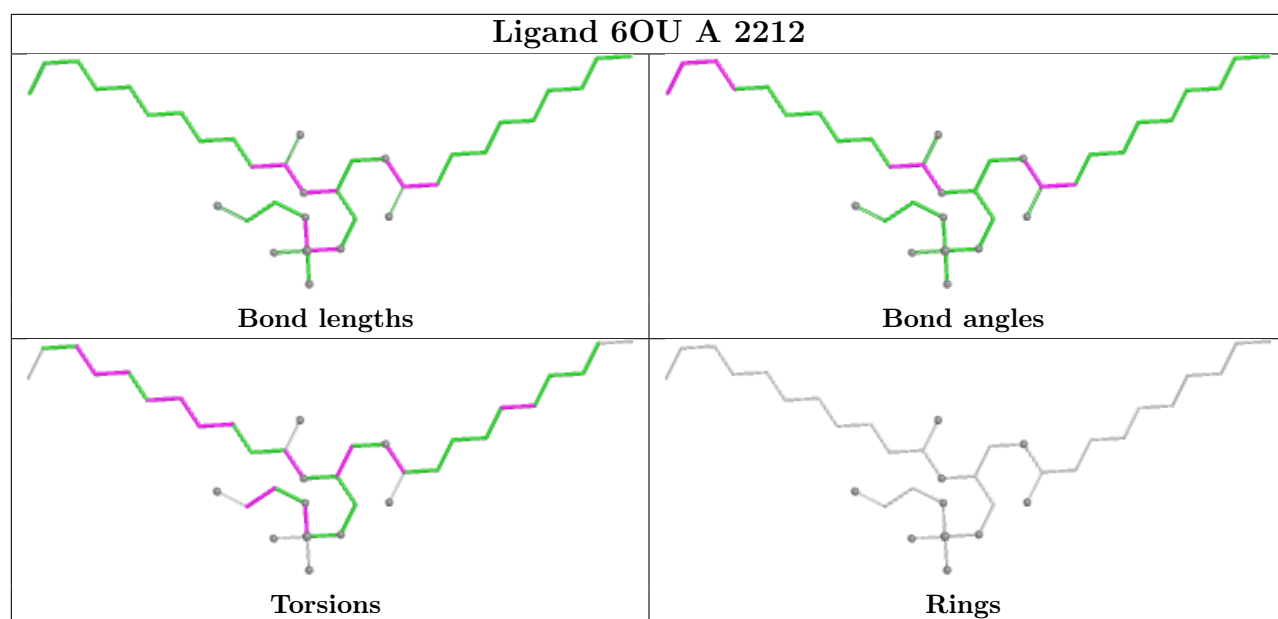


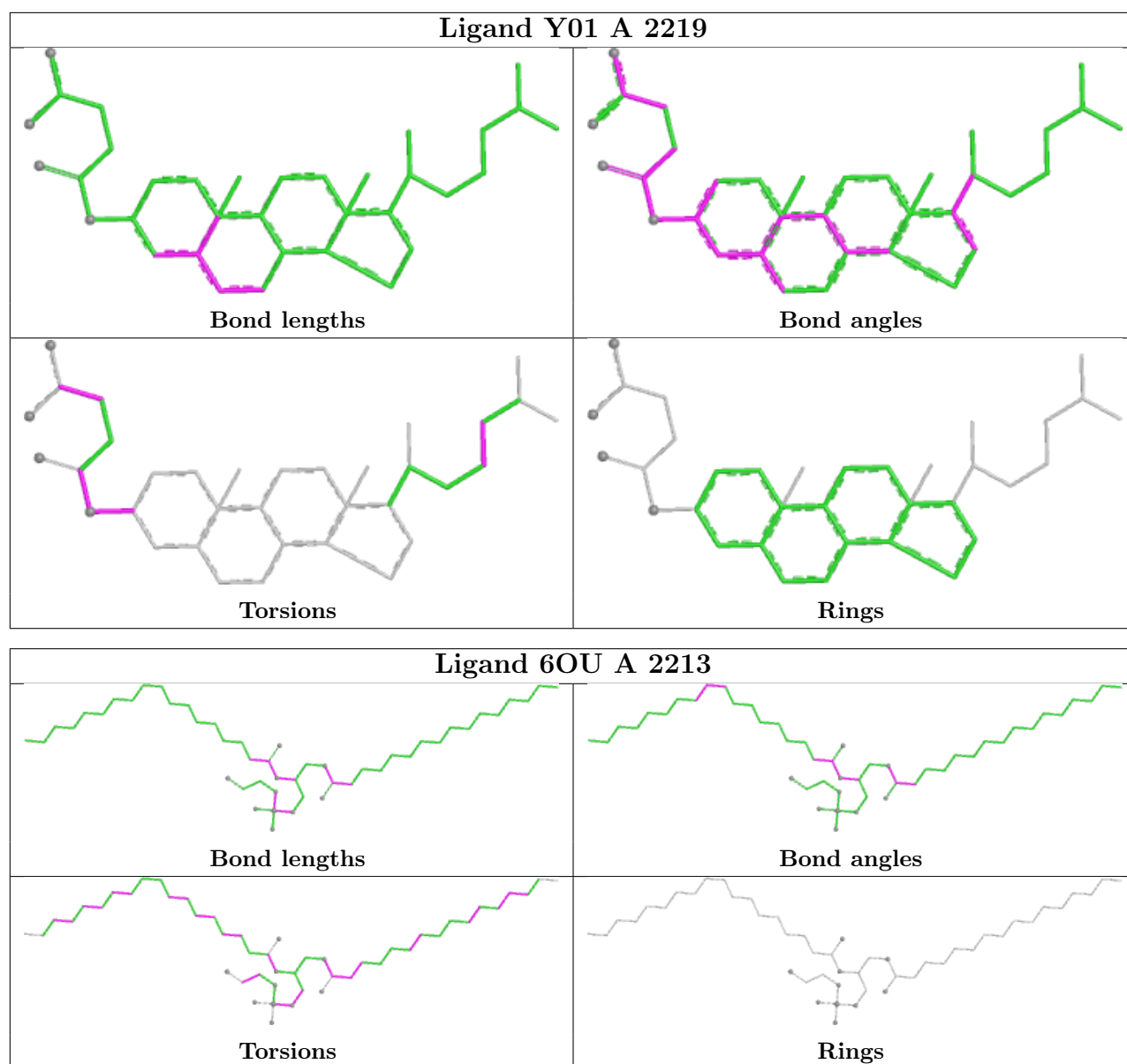


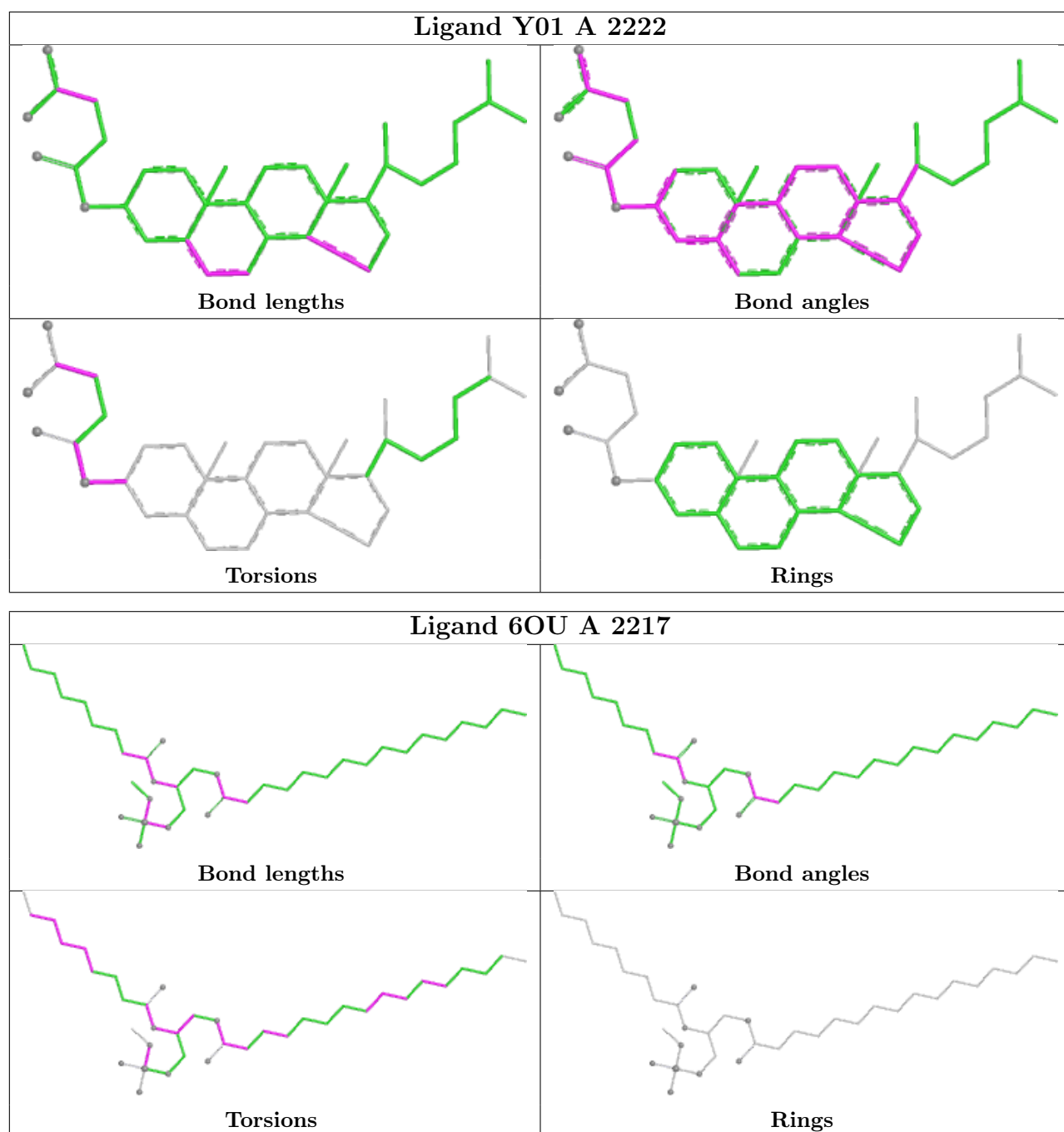


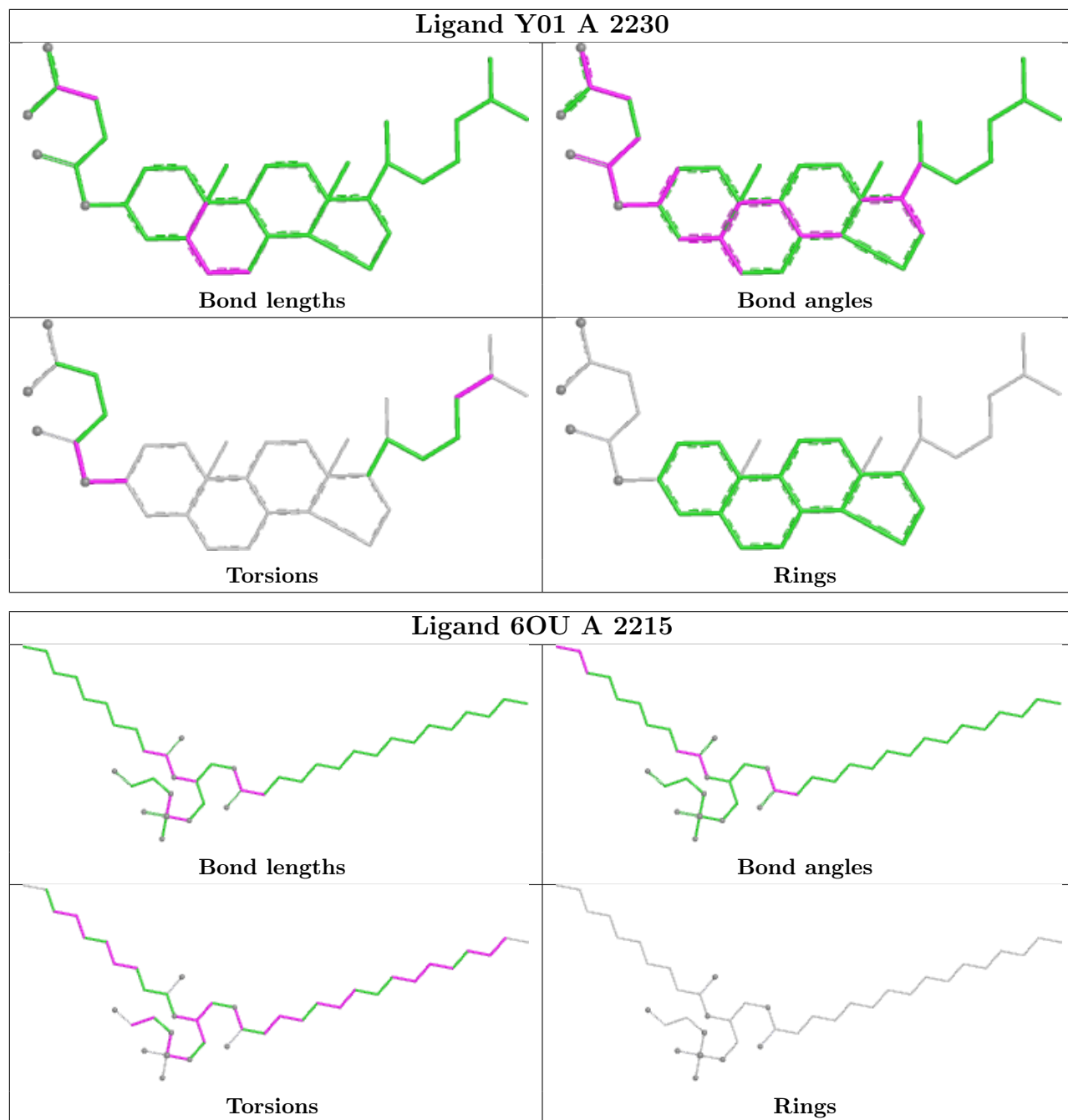


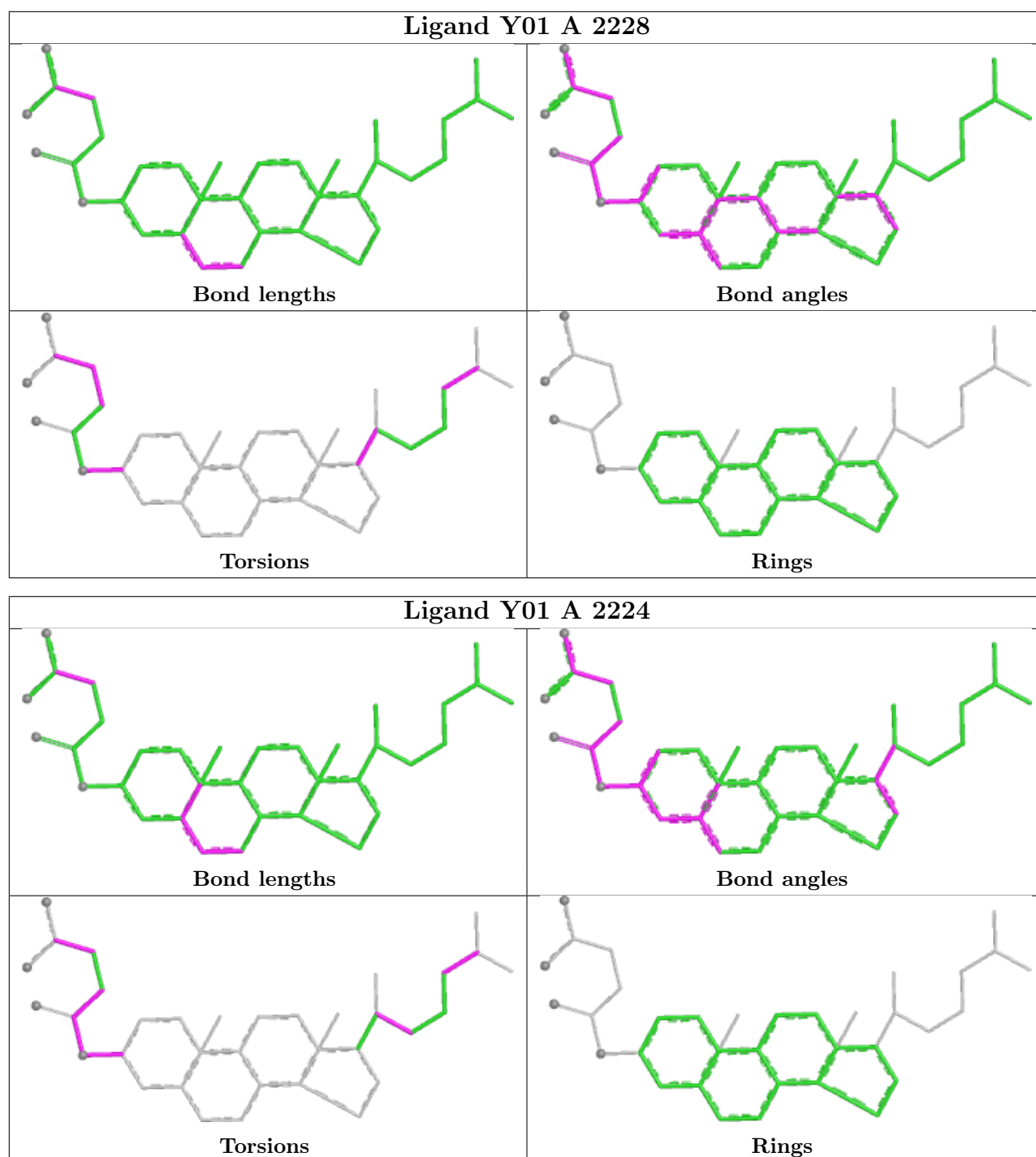












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

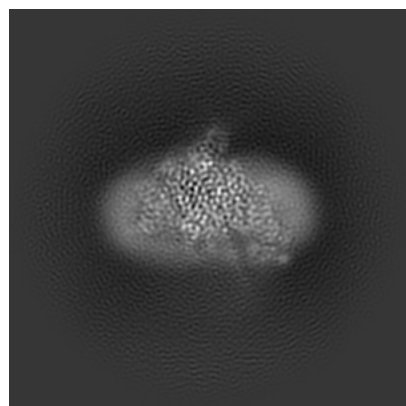
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28887. These allow visual inspection of the internal detail of the map and identification of artifacts.

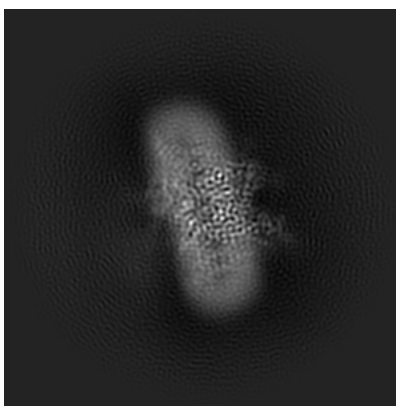
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

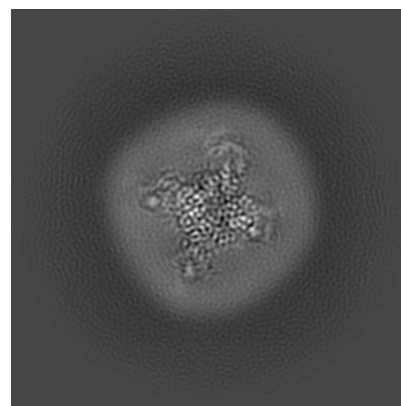
6.1.1 Primary map



X

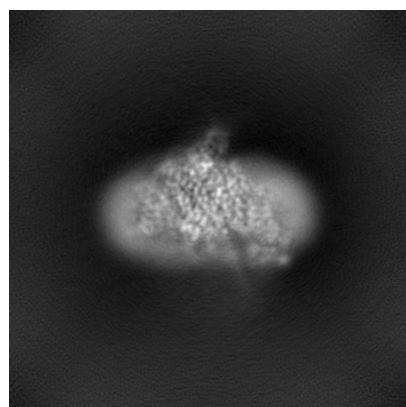


Y

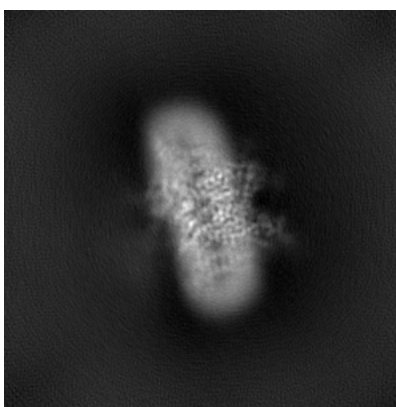


Z

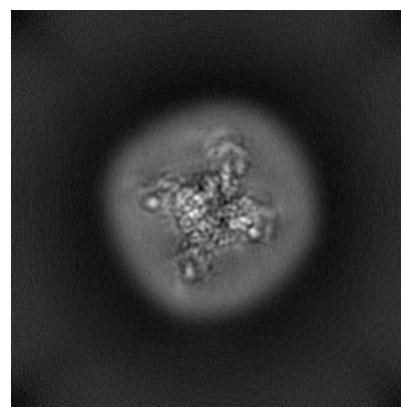
6.1.2 Raw map



X



Y

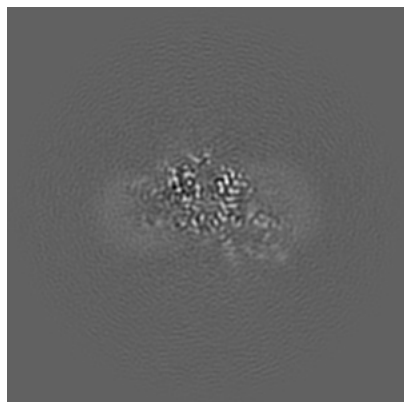


Z

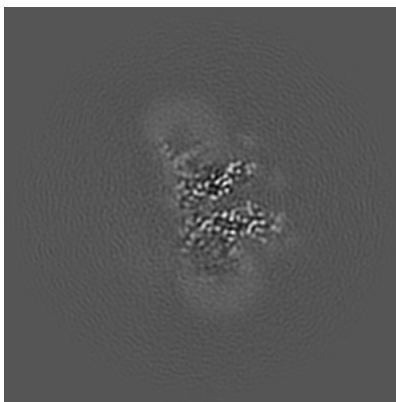
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

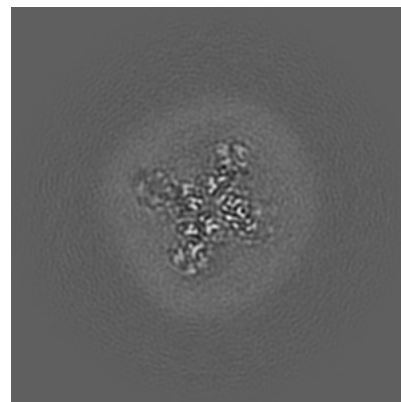
6.2.1 Primary map



X Index: 128

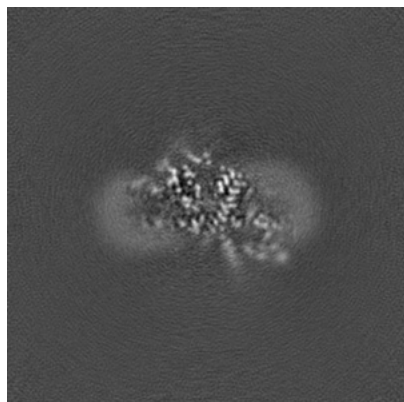


Y Index: 128

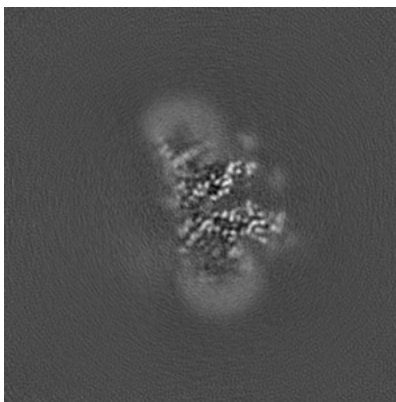


Z Index: 128

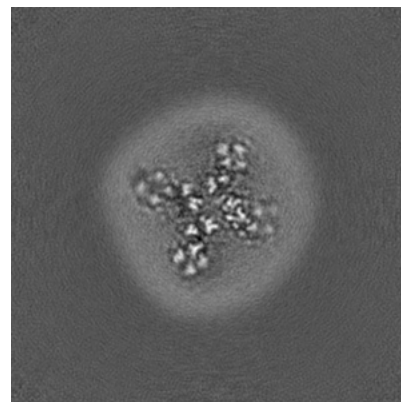
6.2.2 Raw map



X Index: 128



Y Index: 128

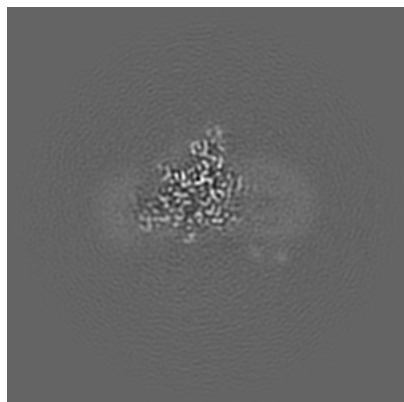


Z Index: 128

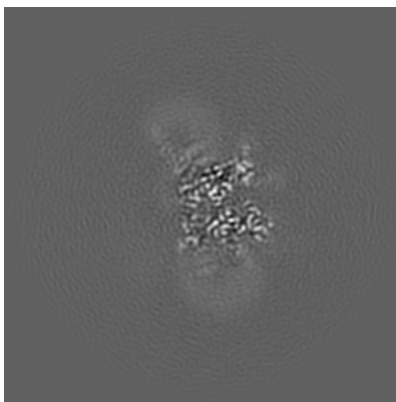
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

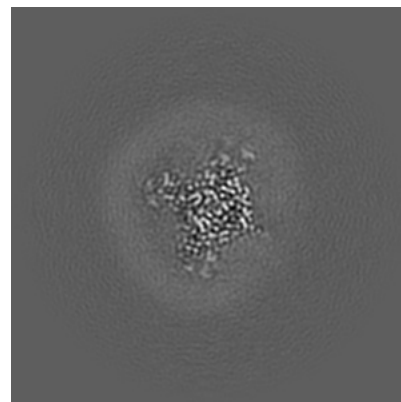
6.3.1 Primary map



X Index: 119

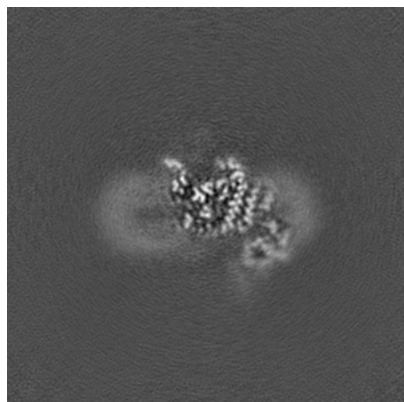


Y Index: 125

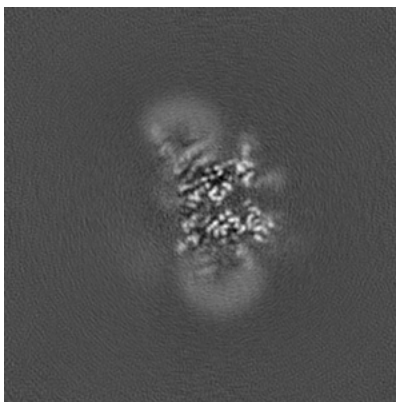


Z Index: 138

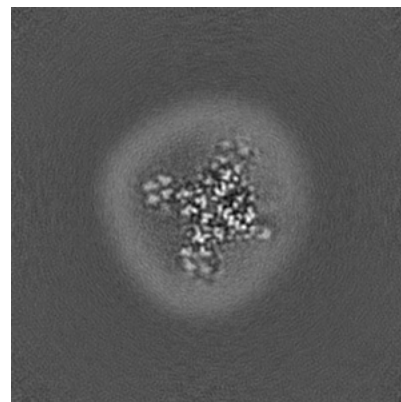
6.3.2 Raw map



X Index: 137



Y Index: 125

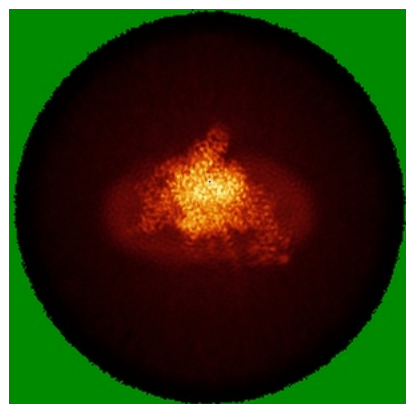


Z Index: 135

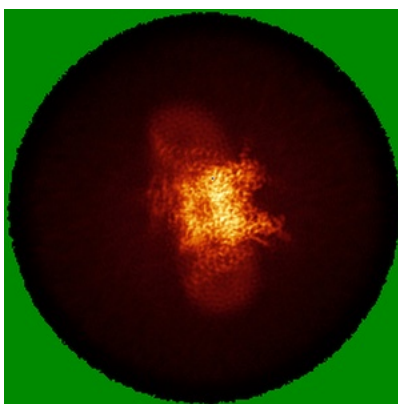
The images above show the largest variance slices of the map in three orthogonal directions.

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

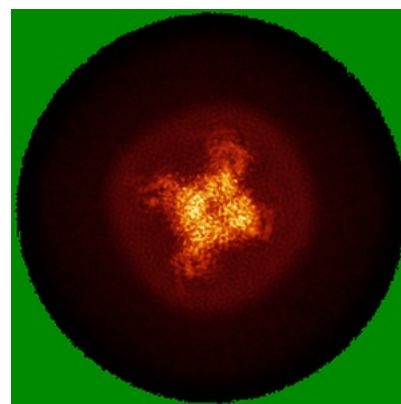
6.4.1 Primary map



X

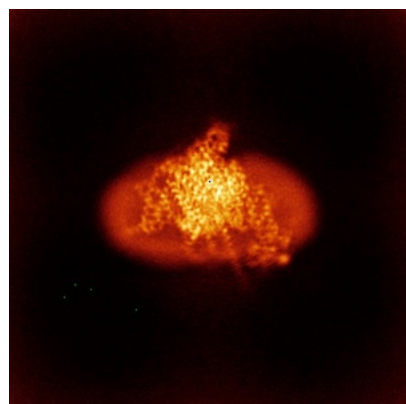


Y

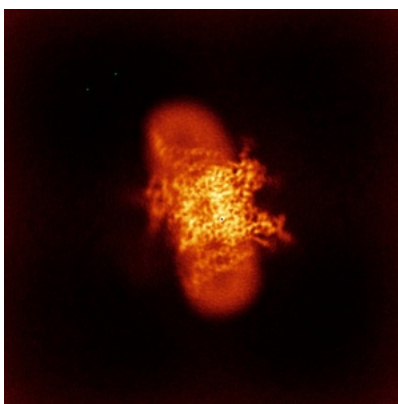


Z

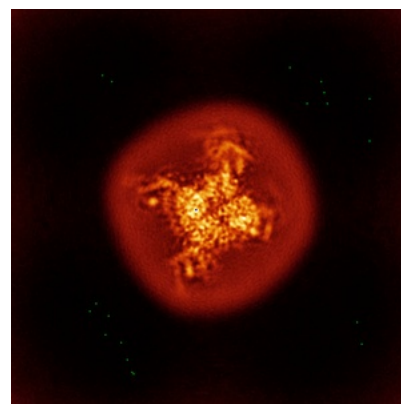
6.4.2 Raw map



X



Y

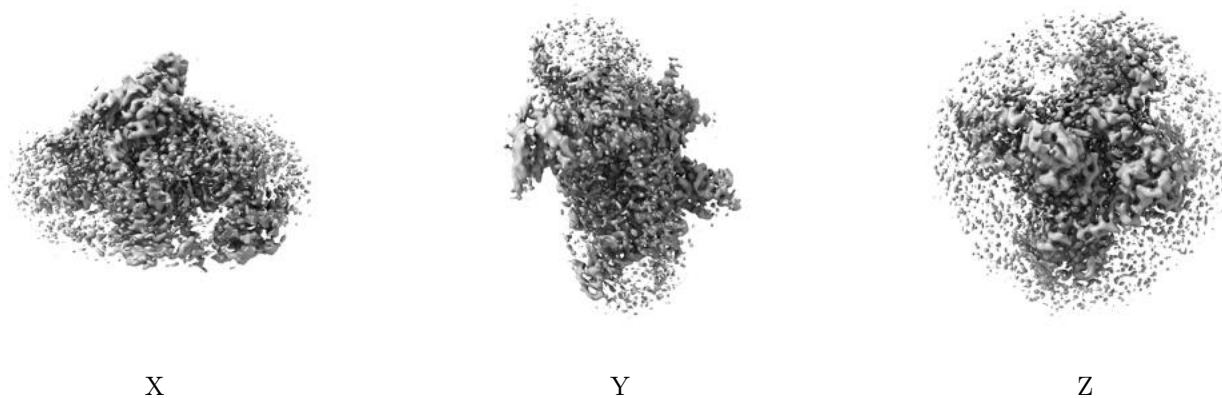


Z

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.

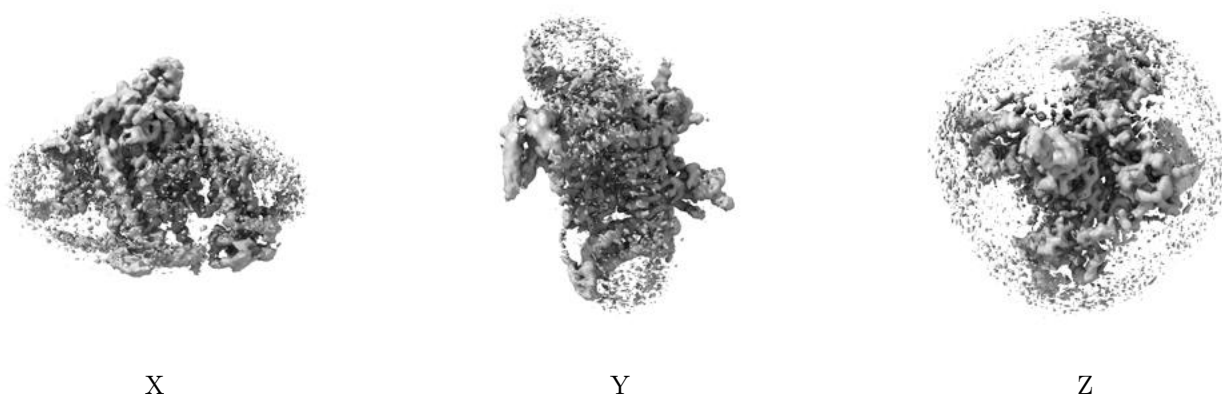
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4171. 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.

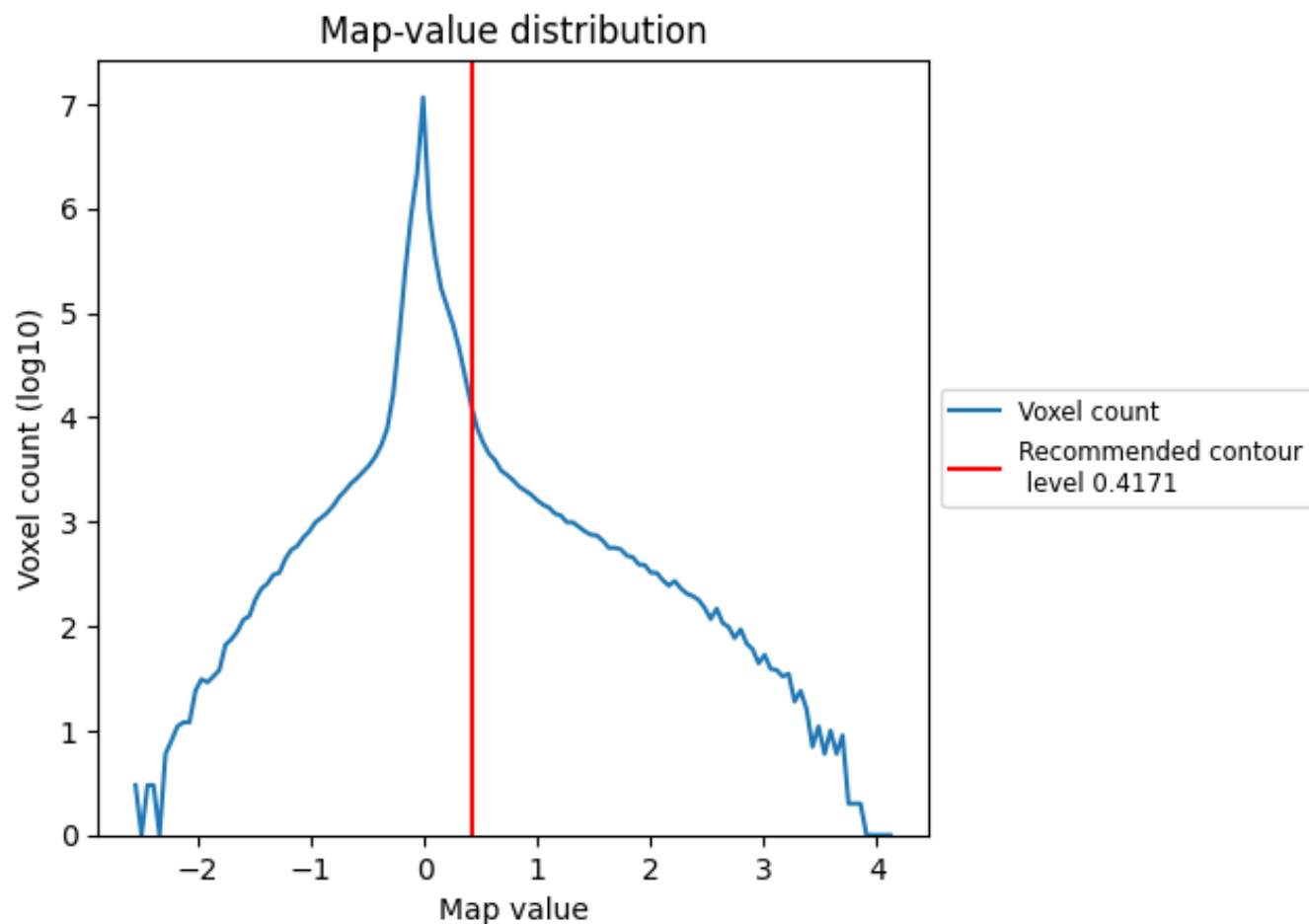
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

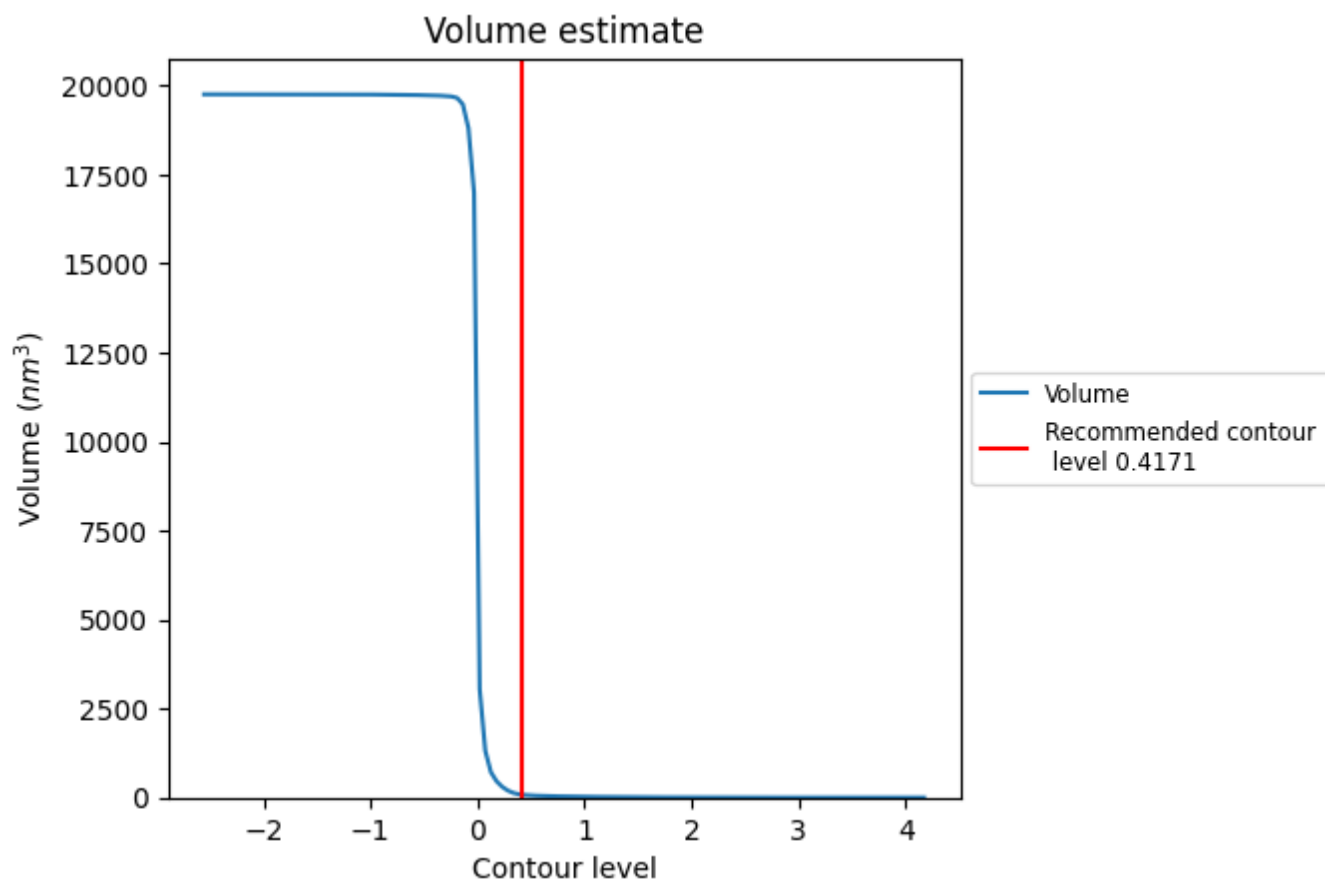
This section contains the results of statistical analysis of the map.

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.

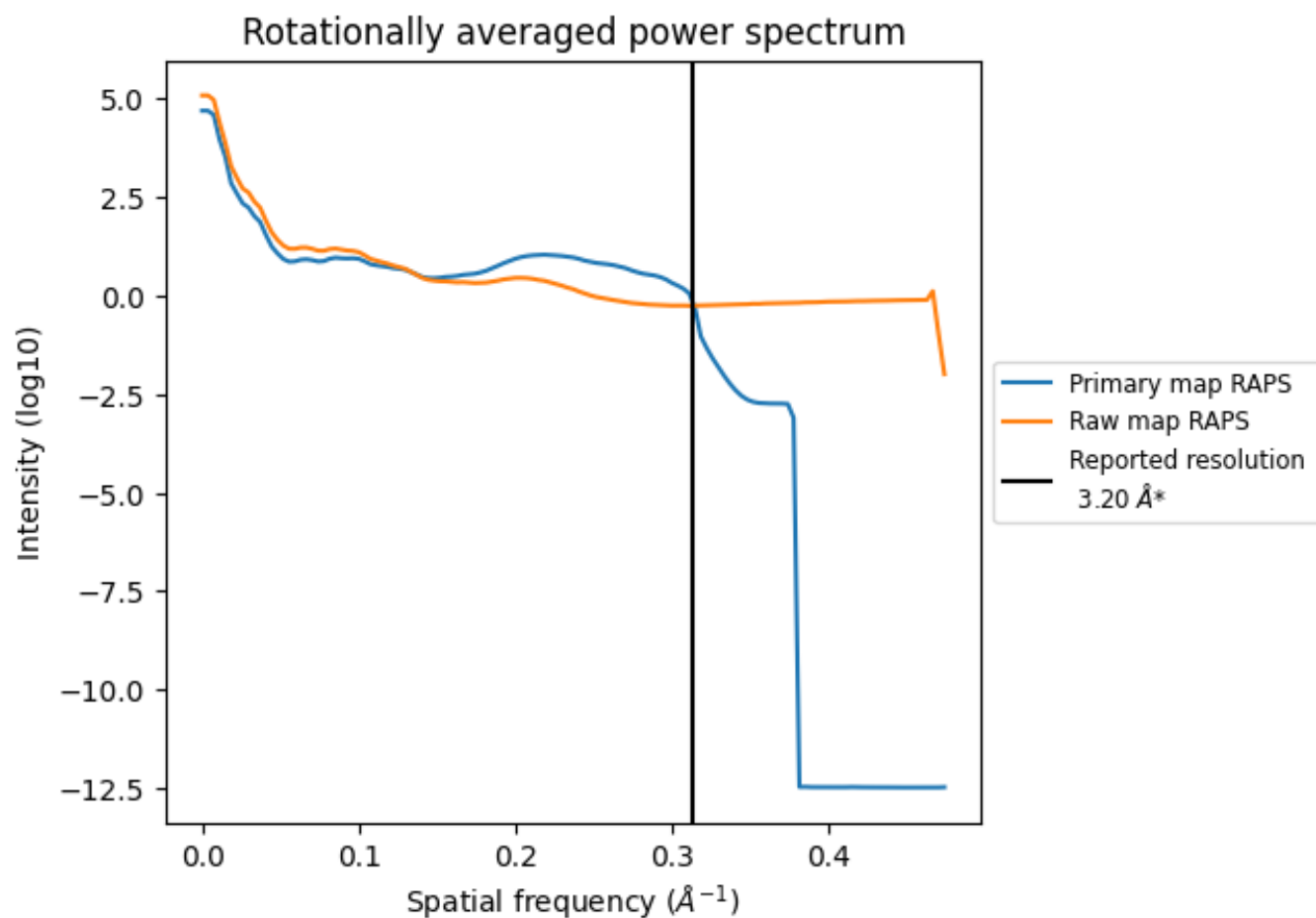
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; this corresponds to an approximate mass of 73 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 ⓘ

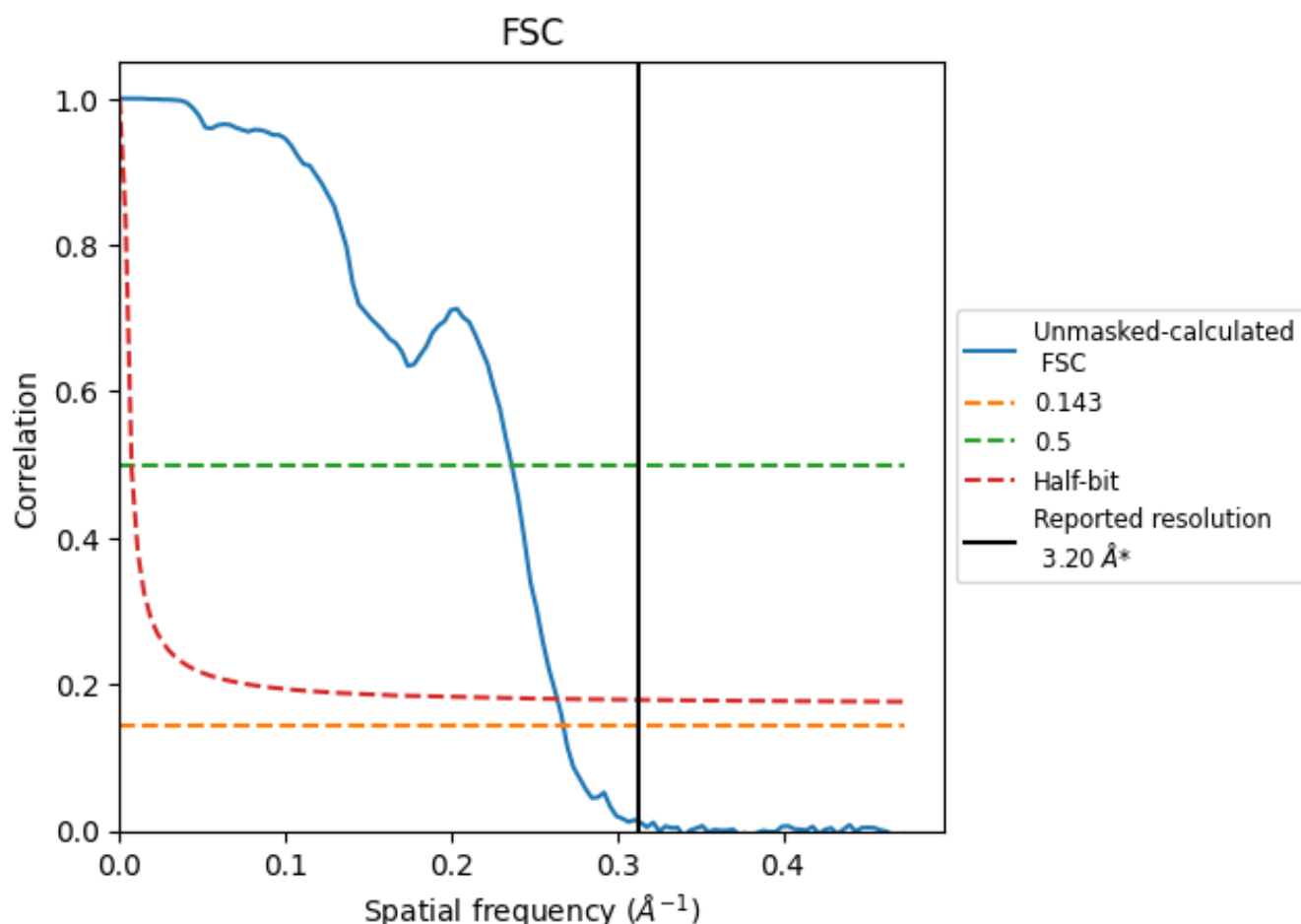


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

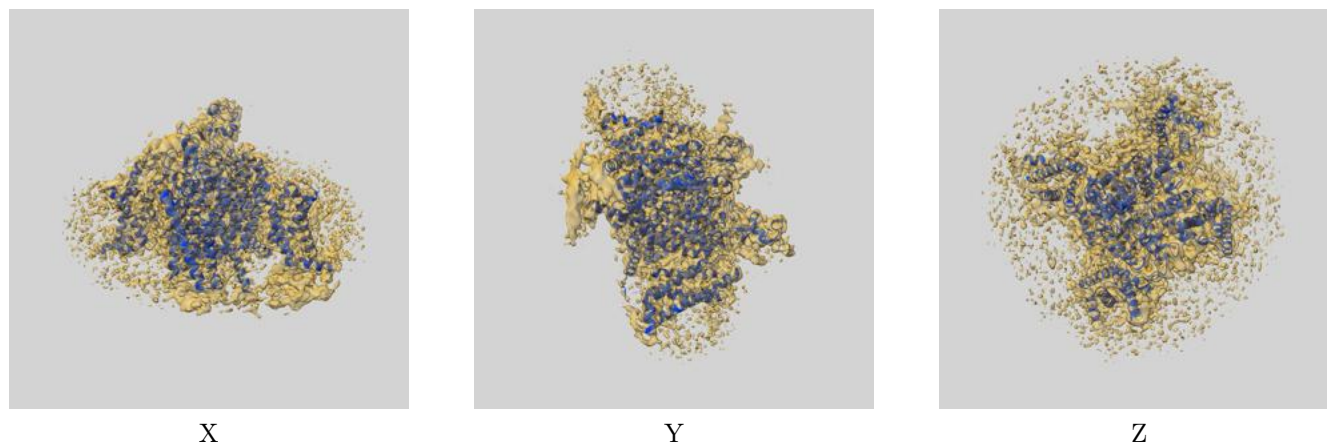
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.23	3.79

*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 3.74 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

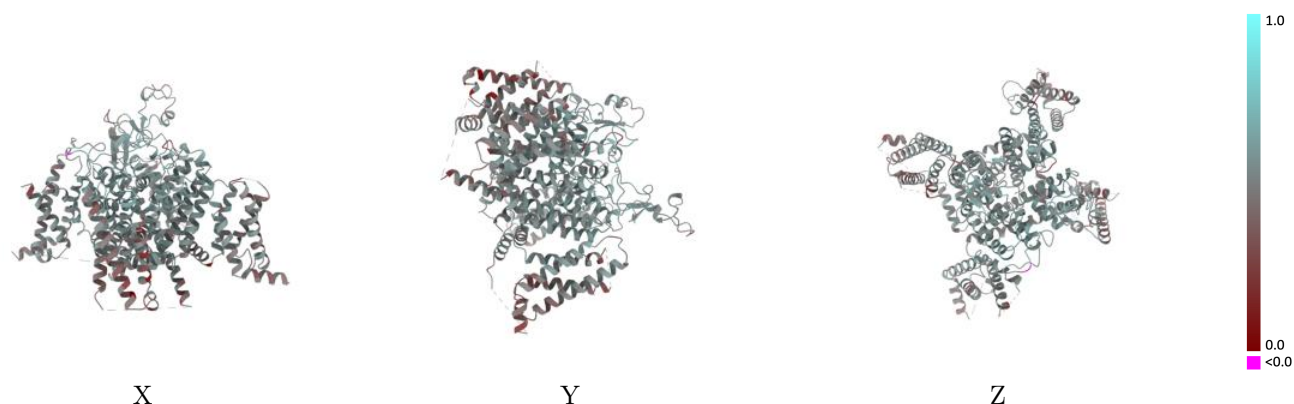
This section contains information regarding the fit between EMDB map EMD-28887 and PDB model 8F6P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



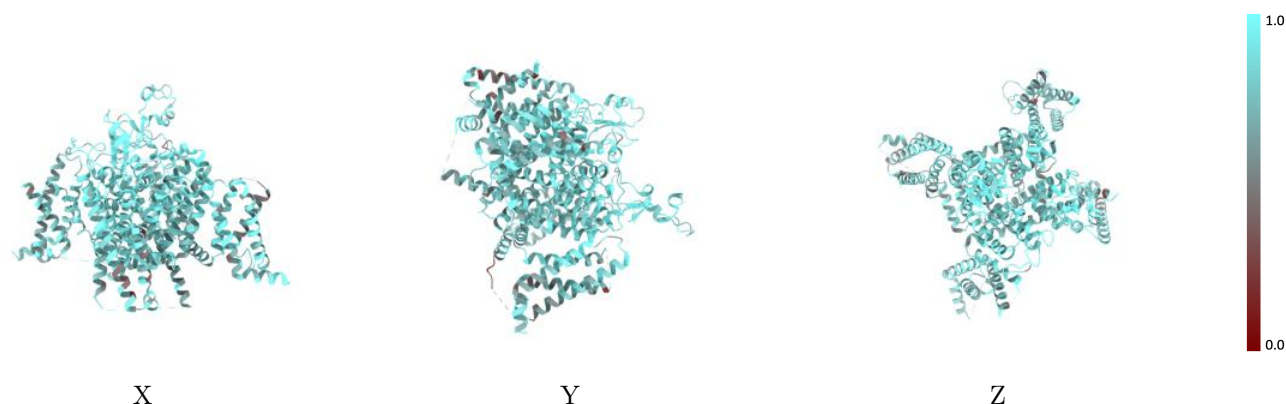
The images above show the 3D surface view of the map at the recommended contour level 0.4171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



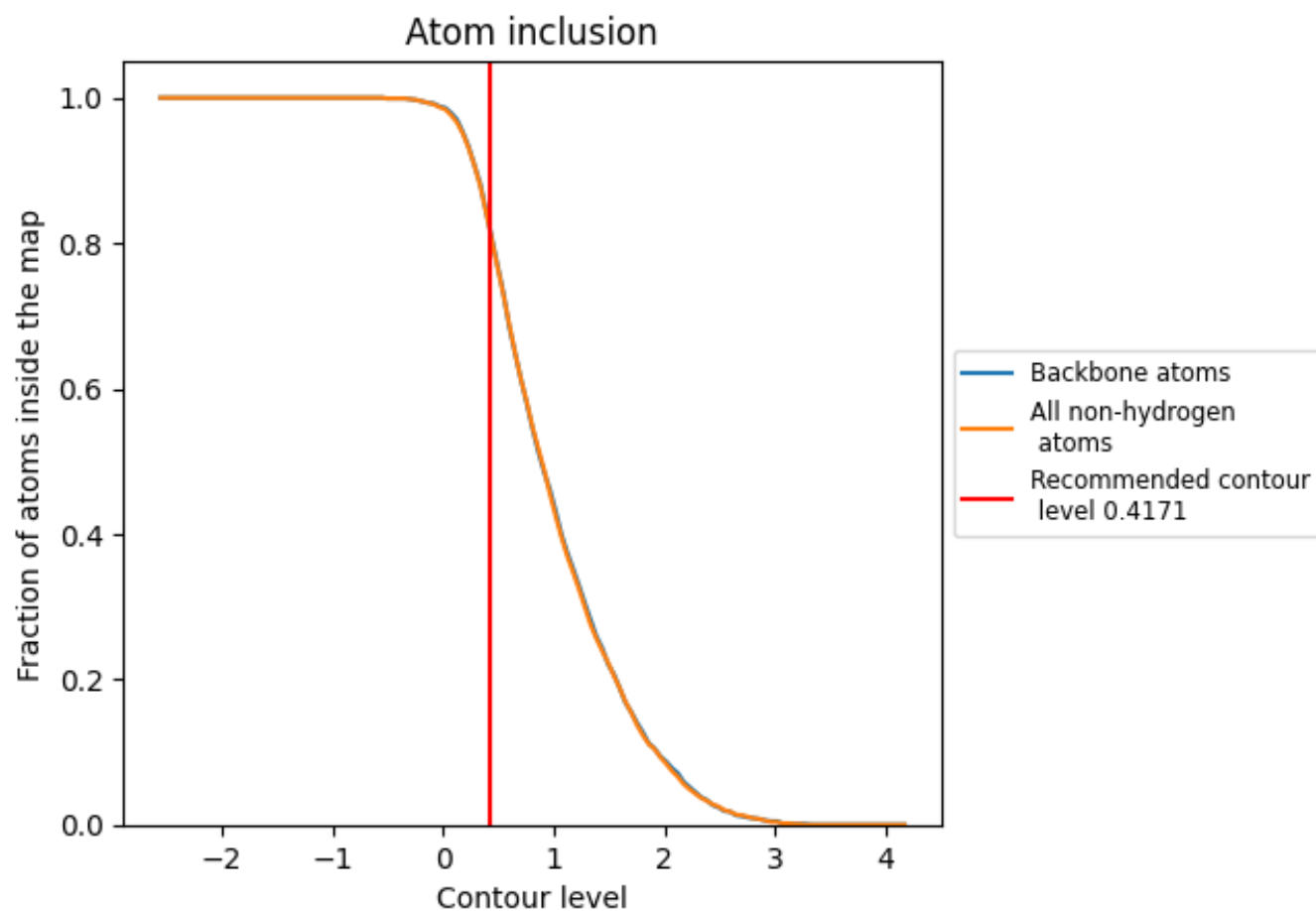
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4171).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.4171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8230	<div></div> 0.5120
A	<div></div> 0.8250	<div></div> 0.5120
B	<div></div> 0.8210	<div></div> 0.4950
C	<div></div> 0.7500	<div></div> 0.4680

