



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:05 AM JST

PDB ID : 7WLK
EMDB ID : EMD-32586
Title : CryoEM structure of human low-voltage activated T-type calcium channel Cav3.3 in complex with Otilonium Bromide(OB)
Authors : He, L.; Yu, Z.; Dong, Y.; Chen, Q.; Zhao, Y.
Deposited on : 2022-01-13
Resolution : 3.60 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

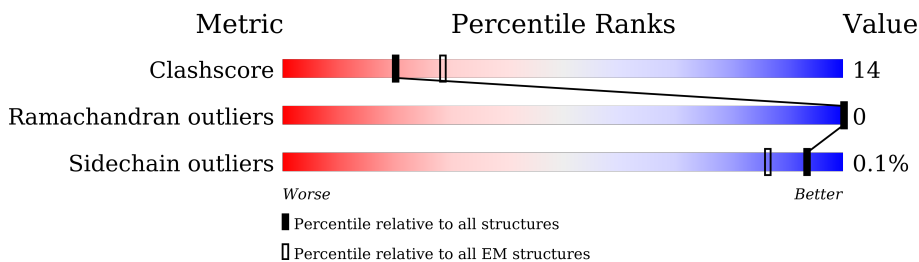
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2223	 36% 15% 49%

2 Entry composition i

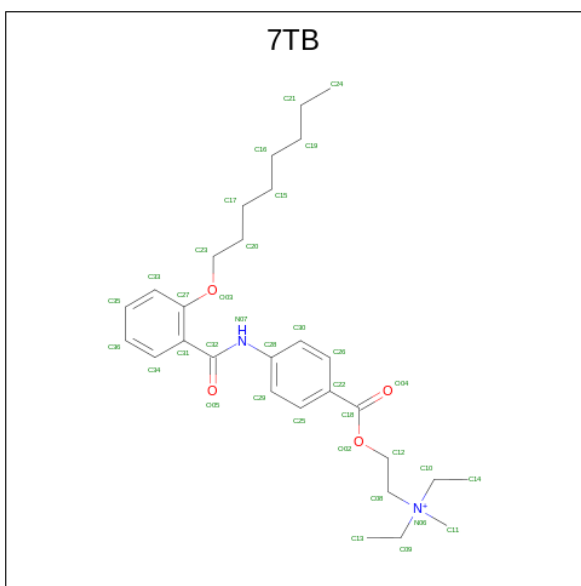
There are 6 unique types of molecules in this entry. The entry contains 9461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 T-type calcium channel subunit alpha-1I.

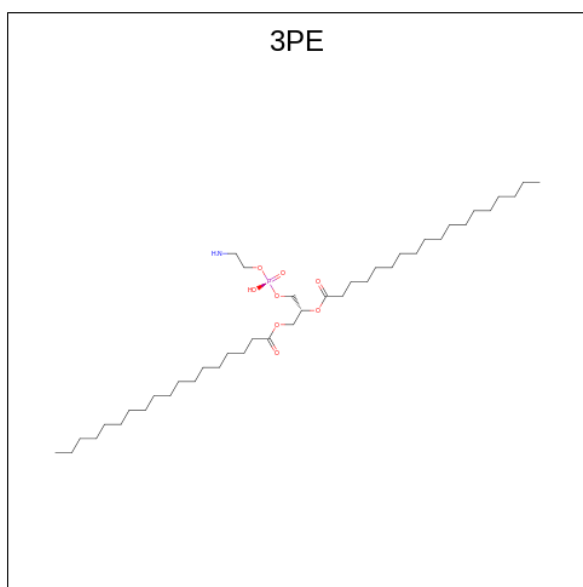
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1135	9111	5979	1499	1555	78	1	0

- Molecule 2 is 2-[diethyl(methyl)- N^+ -azanyljethyl 4-[(2-octoxyphenyl)carbonylamino]benzoate (three-letter code: 7TB) (formula: $\text{C}_{29}\text{H}_{43}\text{N}_2\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	35	29	2	4	0

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).

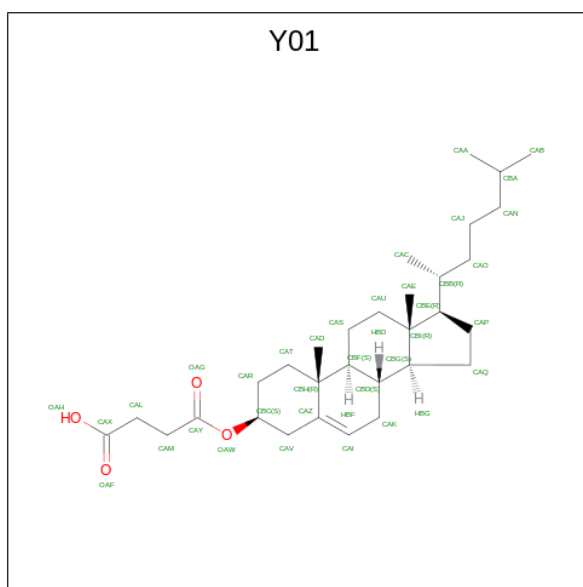


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	89	80	8	1	0
3	A	1	89	80	8	1	0
3	A	1	89	80	8	1	0
3	A	1	89	80	8	1	0
3	A	1	89	80	8	1	0
3	A	1	89	80	8	1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	2	2	2	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	196	179	17	0
5	A	1	196	179	17	0
5	A	1	196	179	17	0
5	A	1	196	179	17	0
5	A	1	196	179	17	0
5	A	1	196	179	17	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
6	A	1	28	16	2	10	0
6	A	1	28	16	2	10	0

PRO
HIS
ALA
ALA
ALA
LEU
ALA
HIS
GLY
LEU
ALA
ARG
SER
PRO
SER
TRP
ALA
ALA
ASP
ARG
SER
LYS
ASP
PRO
PRO
GLY
ARG
ALA
PRO
LEU
PRO
MET
GLY
LEU
GLY
PRO
LEU
ALA
PRO
PRO
PRO
GLN
PRO
LEU
PRO
GLY
GLU
LEU
GLU
PRO
GLY
ASP
ALA
ALA
SER
LYS
ARG
LYS
ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1684039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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, NAG, Y01, 3PE, 7TB

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	0.34	0/9314	0.48	1/12625 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1688	LEU	CA-CB-CG	5.14	127.13	115.30

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	9111	0	9291	246	0
2	A	35	0	0	0	0
3	A	89	0	131	2	0
4	A	2	0	0	0	0
5	A	196	0	279	23	0
6	A	28	0	26	1	0
All	All	9461	0	9727	262	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 14.

All (262) 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:861:LEU:CD1	1:A:1423:LEU:CD2	1.85	1.51
1:A:861:LEU:HD12	1:A:1423:LEU:CD2	1.03	1.49
1:A:861:LEU:CD1	1:A:1423:LEU:HD22	1.51	1.35
1:A:861:LEU:CD1	1:A:1423:LEU:HD21	1.70	1.03
1:A:861:LEU:HD11	1:A:1423:LEU:HD22	1.35	1.02
1:A:1500:ASN:HD21	1:A:1594:ARG:HE	1.14	0.94
1:A:1376:LEU:HD23	1:A:1382:TRP:HB2	1.52	0.92
1:A:861:LEU:HD12	1:A:1423:LEU:HD23	1.52	0.86
1:A:1305:PRO:HG2	1:A:1432:GLU:HG3	1.57	0.85
1:A:332:ASN:HD21	1:A:339:ASN:HD22	1.24	0.83
1:A:1335:CYS:HB3	1:A:1398:GLN:HE22	1.48	0.79
1:A:861:LEU:HD12	1:A:1423:LEU:HD21	0.76	0.76
1:A:332:ASN:ND2	1:A:339:ASN:HD22	1.87	0.73
1:A:266:PRO:HG3	1:A:333:PRO:HB3	1.70	0.72
1:A:1164:GLN:N	1:A:1224:VAL:O	2.22	0.72
1:A:1669:LEU:HD12	5:A:2314:Y01:HAQ2	1.72	0.72
1:A:1668:PHE:HE2	5:A:2314:Y01:HAJ1	1.55	0.72
1:A:660:GLU:OE2	1:A:1326:GLN:NE2	2.22	0.71
1:A:1545:ARG:HA	1:A:1548:LYS:HB2	1.71	0.71
1:A:182:VAL:HG12	1:A:778:ILE:HG22	1.72	0.70
1:A:727:LEU:O	1:A:731:ARG:NH1	2.25	0.70
1:A:680:THR:HG21	1:A:719:ILE:HD11	1.75	0.67
1:A:1527:THR:HG21	1:A:1566:ILE:HG21	1.75	0.67
1:A:1546:PHE:HZ	1:A:1556:LEU:HD22	1.60	0.67
1:A:231:TRP:HA	1:A:234:LEU:HD12	1.79	0.65
1:A:716:ILE:HA	1:A:719:ILE:HD12	1.79	0.65
1:A:70:ASN:OD1	1:A:74:LYS:NZ	2.29	0.65
1:A:1391:ASP:HB3	1:A:1399:PRO:HB2	1.79	0.65
1:A:1480:ILE:HA	1:A:1484:CYS:HB2	1.79	0.64
1:A:1614:GLN:NE2	1:A:1735:ASP:OD2	2.29	0.64
1:A:1613:VAL:HA	1:A:1616:LEU:HD23	1.80	0.64
1:A:277:ILE:HD12	1:A:367:MET:HB3	1.79	0.63
1:A:1555:ASP:OD1	1:A:1597:LYS:NZ	2.32	0.63
1:A:1254:ASP:OD2	1:A:1278:ARG:NE	2.32	0.62
1:A:1345:ASN:HA	1:A:1397:GLN:HA	1.81	0.62
1:A:1472:THR:HB	1:A:1477:ARG:HB2	1.82	0.61
1:A:222:ILE:O	1:A:226:ILE:HG12	2.01	0.61
1:A:1223:VAL:O	1:A:1227:GLY:N	2.33	0.61
1:A:653:ASN:HD21	1:A:737:ARG:HD2	1.66	0.61
1:A:1496:ILE:HG21	1:A:1529:VAL:HG11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:MET:HA	1:A:690:LYS:HE3	1.83	0.60
1:A:1444:GLU:O	1:A:1448:ARG:N	2.33	0.60
1:A:861:LEU:CD1	1:A:1423:LEU:HD23	2.17	0.60
1:A:1500:ASN:O	1:A:1504:MET:HG3	2.02	0.60
1:A:1610:ASP:O	1:A:1613:VAL:N	2.34	0.60
1:A:743:ARG:O	1:A:749:ARG:NH2	2.33	0.60
1:A:680:THR:HA	1:A:683:PHE:HD1	1.66	0.59
1:A:1530:PHE:HB3	1:A:1559:VAL:HG22	1.84	0.58
1:A:1557:ALA:O	1:A:1561:LEU:HG	2.04	0.58
1:A:1378:SER:HA	3:A:2302:3PE:H32	1.85	0.58
1:A:1367:GLY:HA3	5:A:2310:Y01:HBG	1.86	0.58
1:A:1176:VAL:O	1:A:1180:ILE:HG13	2.03	0.57
1:A:731:ARG:HG3	1:A:734:ARG:NH1	2.18	0.57
1:A:1626:PHE:CE2	1:A:1630:PHE:HE2	2.23	0.57
1:A:809:TRP:HA	1:A:812:VAL:HG12	1.86	0.57
1:A:1293:LYS:O	1:A:1297:GLU:HG2	2.05	0.57
1:A:1283:LEU:HD13	1:A:1632:ILE:HD11	1.87	0.56
1:A:1281:ARG:O	1:A:1283:LEU:N	2.35	0.56
1:A:1582:THR:O	1:A:1586:ILE:HG12	2.04	0.56
1:A:1360:LYS:NZ	1:A:1688:LEU:O	2.36	0.56
1:A:90:LEU:O	1:A:94:VAL:HG23	2.06	0.56
1:A:1475:HIS:O	1:A:1477:ARG:NH1	2.39	0.55
1:A:1452:LYS:HA	1:A:1455:ARG:HE	1.71	0.55
1:A:375:PHE:O	1:A:379:ILE:HG12	2.06	0.55
1:A:1377:ALA:HB1	1:A:1418:VAL:HG11	1.88	0.55
1:A:1655:MET:HA	1:A:1659:ALA:HB3	1.89	0.55
1:A:729:VAL:HG13	3:A:2315:3PE:H362	1.89	0.55
1:A:1471:ALA:O	1:A:1475:HIS:ND1	2.40	0.54
1:A:153:LEU:O	1:A:157:ILE:HD12	2.07	0.54
1:A:802:LYS:HD3	1:A:816:GLN:HE22	1.71	0.54
1:A:1500:ASN:ND2	1:A:1594:ARG:HE	1.95	0.54
1:A:1500:ASN:HD21	1:A:1594:ARG:NE	1.95	0.54
1:A:123:PHE:HE2	1:A:161:GLY:HA3	1.73	0.54
1:A:1456:ARG:HA	1:A:1459:LYS:HD2	1.88	0.54
1:A:820:GLN:HB3	1:A:846:MET:HE1	1.90	0.53
6:A:2311:NAG:H3	6:A:2311:NAG:H83	1.89	0.53
1:A:1238:SER:OG	1:A:1241:ASN:OD1	2.17	0.53
1:A:1492:PHE:O	1:A:1496:ILE:HG12	2.09	0.53
1:A:237:ASN:HB3	1:A:328:THR:HG22	1.91	0.52
1:A:1726:VAL:O	1:A:1730:MET:HG2	2.09	0.52
1:A:1190:GLU:HG2	1:A:1204:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1706:SER:OG	1:A:1707:PRO:HD3	2.09	0.52
1:A:1331:LYS:NZ	1:A:1394:ALA:HA	2.25	0.52
1:A:676:ASN:ND2	1:A:734:ARG:HH21	2.09	0.51
1:A:228:VAL:O	1:A:232:ALA:HB2	2.11	0.51
1:A:214:LEU:HD22	1:A:1605:MET:HE3	1.92	0.51
1:A:236:ARG:HG2	1:A:332:ASN:HB3	1.92	0.51
1:A:1609:LEU:O	1:A:1613:VAL:HG23	2.11	0.51
1:A:120:ASP:O	1:A:124:ILE:HG12	2.10	0.50
1:A:859:ALA:HA	1:A:862:VAL:HG22	1.92	0.50
1:A:1394:ALA:HB3	1:A:1397:GLN:NE2	2.27	0.50
1:A:350:ILE:O	1:A:354:ILE:HG12	2.10	0.50
1:A:1506:LEU:O	1:A:1508:HIS:ND1	2.39	0.50
1:A:1530:PHE:CE2	1:A:1594:ARG:HD2	2.47	0.50
1:A:1532:LEU:O	1:A:1536:LEU:HG	2.11	0.50
1:A:686:GLU:OE2	1:A:690:LYS:HD3	2.12	0.50
1:A:1503:THR:HA	1:A:1506:LEU:HD12	1.92	0.50
1:A:1335:CYS:HB3	1:A:1398:GLN:NE2	2.24	0.50
1:A:245:PHE:HE1	1:A:322:TYR:HD2	1.61	0.49
1:A:1200:GLU:O	1:A:1204:LEU:HG	2.12	0.49
1:A:363:MET:HG3	1:A:378:PHE:CG	2.47	0.49
1:A:668:LEU:O	1:A:672:LEU:HD23	2.13	0.49
1:A:1530:PHE:HE2	1:A:1594:ARG:HD2	1.78	0.49
1:A:70:ASN:O	1:A:74:LYS:NZ	2.44	0.49
1:A:157:ILE:HG21	1:A:184:ARG:HG3	1.95	0.49
1:A:1218:GLU:O	1:A:1222:LYS:HG2	2.13	0.49
1:A:1633:TYR:HD1	1:A:1709:TYR:CE1	2.30	0.49
1:A:1244:ASP:OD1	1:A:1284:ARG:HG2	2.13	0.49
1:A:1279:THR:HG21	1:A:1639:GLU:HG3	1.95	0.49
1:A:1469:TYR:HD2	1:A:1473:TYR:CE2	2.31	0.49
1:A:670:ASN:HA	1:A:673:GLU:CD	2.33	0.48
1:A:88:VAL:HG21	1:A:125:PHE:CE1	2.47	0.48
1:A:653:ASN:ND2	1:A:737:ARG:HD2	2.27	0.48
1:A:1389:GLY:HA3	1:A:1411:PHE:HE2	1.78	0.48
1:A:1480:ILE:HG22	1:A:1540:ALA:HB2	1.95	0.48
5:A:2310:Y01:HAE2	5:A:2310:Y01:HBB	1.71	0.48
1:A:137:LEU:HD12	1:A:145:TYR:HA	1.95	0.48
1:A:699:TYR:HD2	1:A:700:LEU:HD22	1.78	0.48
1:A:1219:MET:SD	1:A:1248:VAL:HG11	2.53	0.48
1:A:630:ARG:HG2	1:A:693:ALA:HA	1.95	0.48
1:A:1626:PHE:CZ	1:A:1630:PHE:HE2	2.31	0.48
1:A:332:ASN:HB2	1:A:333:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:LEU:HD23	1:A:1723:ASN:ND2	2.29	0.48
1:A:1354:TYR:O	1:A:1355:ARG:HG3	2.13	0.48
1:A:699:TYR:CZ	1:A:705:ASN:HB3	2.49	0.48
1:A:1523:ASN:O	1:A:1527:THR:HG23	2.14	0.48
1:A:89:ILE:HG21	1:A:188:ALA:HB2	1.96	0.47
1:A:1481:HIS:O	1:A:1485:THR:OG1	2.18	0.47
1:A:754:VAL:O	1:A:758:THR:HG23	2.14	0.47
1:A:338:ILE:HD12	1:A:349:VAL:HG22	1.96	0.47
1:A:86:MET:HG2	1:A:191:ARG:HB3	1.97	0.47
1:A:713:ILE:HA	1:A:716:ILE:HG12	1.96	0.47
1:A:1554:LEU:O	1:A:1558:ILE:HG12	2.14	0.47
1:A:686:GLU:HG3	1:A:690:LYS:HD3	1.96	0.47
1:A:1386:MET:O	1:A:1390:LEU:HG	2.14	0.47
1:A:267:PHE:CE2	1:A:283:ILE:HG12	2.50	0.47
1:A:402:SER:O	1:A:406:GLN:HG2	2.15	0.47
1:A:332:ASN:OD1	1:A:336:GLY:HA2	2.14	0.47
1:A:816:GLN:NE2	1:A:1383:VAL:HG21	2.30	0.47
1:A:1585:ARG:O	1:A:1589:VAL:HG12	2.14	0.47
1:A:1192:PRO:HG3	1:A:1642:GLY:HA3	1.97	0.46
1:A:1379:LYS:HB2	1:A:1379:LYS:HE3	1.59	0.46
1:A:259:PRO:HD2	1:A:265:MET:O	2.15	0.46
1:A:1250:VAL:HG11	1:A:1277:LEU:HB3	1.97	0.46
1:A:1691:CYS:H	1:A:1698:CYS:HB2	1.79	0.46
1:A:1479:LEU:H	1:A:1479:LEU:HD23	1.81	0.46
1:A:1493:ILE:O	1:A:1497:ILE:HG12	2.15	0.46
5:A:2308:Y01:HAE2	5:A:2308:Y01:HBB	1.75	0.46
1:A:708:ASP:OD1	1:A:740:LYS:HD3	2.15	0.46
5:A:2314:Y01:HAP1	5:A:2314:Y01:HAO2	1.38	0.46
1:A:85:SER:O	1:A:89:ILE:HG12	2.15	0.46
1:A:136:ALA:O	1:A:137:LEU:HD23	2.15	0.46
1:A:1360:LYS:HZ1	1:A:1689:ARG:HA	1.81	0.46
1:A:378:PHE:O	1:A:382:ILE:HG12	2.16	0.46
1:A:840:LEU:HB2	5:A:2312:Y01:HAQ2	1.98	0.46
1:A:126:PHE:HE2	1:A:184:ARG:HD3	1.80	0.46
1:A:1444:GLU:HA	1:A:1447:ARG:HB2	1.98	0.46
1:A:1168:ALA:O	1:A:1169:HIS:ND1	2.45	0.46
1:A:1220:THR:HA	1:A:1223:VAL:HG12	1.98	0.46
1:A:1448:ARG:O	1:A:1452:LYS:N	2.43	0.46
1:A:1580:ASN:OD1	1:A:1582:THR:OG1	2.25	0.46
1:A:321:ARG:HG3	1:A:322:TYR:HD1	1.81	0.46
1:A:224:GLY:O	1:A:228:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:TYR:CD2	1:A:743:ARG:HG3	2.52	0.45
1:A:1591:ARG:O	1:A:1594:ARG:HG3	2.16	0.45
1:A:861:LEU:HB2	1:A:1427:VAL:HG21	1.98	0.45
1:A:1668:PHE:CE2	5:A:2314:Y01:HAJ1	2.43	0.45
5:A:2309:Y01:HAO1	5:A:2309:Y01:HAP1	1.31	0.45
5:A:2316:Y01:HAO2	5:A:2316:Y01:HAP1	1.41	0.45
1:A:683:PHE:HD2	1:A:740:LYS:HZ1	1.62	0.45
1:A:763:ALA:O	1:A:767:MET:HG2	2.17	0.45
1:A:1667:ALA:O	1:A:1671:LEU:HD23	2.17	0.45
5:A:2314:Y01:HAR2	5:A:2316:Y01:HAD2	1.98	0.45
1:A:1246:PHE:O	1:A:1250:VAL:HG23	2.17	0.45
1:A:245:PHE:CE2	1:A:247:ILE:HB	2.52	0.45
1:A:280:CYS:SG	1:A:326:CYS:HB3	2.57	0.45
1:A:731:ARG:HG3	1:A:734:ARG:HH11	1.79	0.45
5:A:2312:Y01:HBB	5:A:2312:Y01:HAE2	1.59	0.45
1:A:1717:ALA:O	1:A:1721:LEU:HG	2.18	0.44
1:A:818:LEU:HA	1:A:818:LEU:HD23	1.83	0.44
1:A:1430:VAL:HG22	1:A:1726:VAL:HG22	1.98	0.44
1:A:92:ASN:ND2	1:A:184:ARG:HD2	2.32	0.44
1:A:1390:LEU:HD23	1:A:1407:MET:HB2	2.00	0.44
1:A:1499:LEU:HA	1:A:1502:VAL:HG22	1.99	0.44
5:A:2308:Y01:HAO1	5:A:2308:Y01:HAP1	1.76	0.44
1:A:1270:VAL:O	1:A:1274:LEU:HD23	2.17	0.44
1:A:392:LEU:HD23	1:A:392:LEU:HA	1.91	0.44
1:A:1232:GLU:HA	1:A:1237:ARG:NE	2.32	0.44
5:A:2309:Y01:HAE2	5:A:2309:Y01:HBB	1.60	0.44
1:A:777:SER:O	1:A:781:MET:HG3	2.17	0.44
1:A:642:PHE:HE2	1:A:686:GLU:OE1	2.01	0.43
1:A:1527:THR:HG22	1:A:1562:SER:OG	2.17	0.43
1:A:1618:GLN:O	1:A:1622:LEU:HD23	2.18	0.43
5:A:2316:Y01:HAC2	5:A:2316:Y01:HAJ2	1.65	0.43
1:A:668:LEU:HA	1:A:671:ILE:HD12	1.99	0.43
1:A:834:THR:OG1	1:A:835:SER:N	2.51	0.43
1:A:1183:ASN:O	1:A:1187:ILE:HG13	2.17	0.43
1:A:353:VAL:CG1	1:A:362:ILE:HD11	2.47	0.43
1:A:111:ARG:O	1:A:115:LEU:HG	2.18	0.43
1:A:853:LEU:HD23	1:A:853:LEU:HA	1.81	0.43
5:A:2314:Y01:HAE2	5:A:2314:Y01:HBB	1.79	0.43
1:A:715:SER:O	1:A:719:ILE:HG13	2.18	0.43
1:A:676:ASN:HD22	1:A:734:ARG:HH21	1.66	0.43
1:A:1181:PHE:CE1	5:A:2316:Y01:HAB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:ARG:NH2	1:A:1639:GLU:OE2	2.45	0.43
1:A:1591:ARG:HG2	1:A:1594:ARG:NH1	2.34	0.43
1:A:1563:VAL:HA	1:A:1566:ILE:HG12	2.00	0.43
1:A:1588:ARG:O	1:A:1591:ARG:HB2	2.19	0.43
1:A:690:LYS:HG3	1:A:699:TYR:HE1	1.84	0.43
1:A:238:ARG:HH11	1:A:332:ASN:HA	1.84	0.42
5:A:2312:Y01:HAO2	5:A:2312:Y01:HAP1	1.23	0.42
5:A:2316:Y01:HAE2	5:A:2316:Y01:HBB	1.71	0.42
1:A:1308:ASN:O	1:A:1312:ILE:HG13	2.20	0.42
1:A:831:MET:SD	1:A:839:SER:HB3	2.59	0.42
1:A:1181:PHE:HE1	5:A:2316:Y01:HAB2	1.84	0.42
1:A:1668:PHE:CD2	5:A:2314:Y01:HBE	2.54	0.42
1:A:376:ILE:HD12	1:A:376:ILE:H	1.85	0.42
1:A:1389:GLY:HA3	1:A:1411:PHE:CE2	2.54	0.42
5:A:2308:Y01:HAJ1	5:A:2308:Y01:HAC3	1.69	0.42
1:A:245:PHE:HE1	1:A:322:TYR:CD2	2.38	0.42
1:A:650:ILE:HG12	1:A:683:PHE:HE2	1.85	0.42
1:A:709:SER:HA	1:A:712:VAL:HG12	2.01	0.42
1:A:707:PHE:O	1:A:711:ILE:HG12	2.20	0.42
1:A:113:LYS:O	1:A:117:VAL:HG23	2.18	0.42
1:A:126:PHE:CE2	1:A:184:ARG:HD3	2.55	0.42
1:A:142:LYS:HE3	1:A:142:LYS:HB3	1.88	0.42
1:A:398:ALA:HA	1:A:859:ALA:HB2	2.01	0.42
1:A:1191:ARG:HG3	1:A:1193:GLN:HB3	2.02	0.42
1:A:1212:THR:O	1:A:1216:VAL:HG23	2.19	0.42
1:A:1288:ARG:HG3	1:A:1288:ARG:HH11	1.83	0.42
1:A:88:VAL:HG21	1:A:125:PHE:CD1	2.55	0.42
1:A:690:LYS:HG3	1:A:699:TYR:CE1	2.55	0.42
1:A:208:MET:SD	1:A:208:MET:N	2.93	0.41
1:A:1434:PHE:HA	1:A:1730:MET:HE3	2.01	0.41
1:A:1688:LEU:O	1:A:1688:LEU:HD12	2.19	0.41
1:A:132:LEU:HA	1:A:135:VAL:HG12	2.02	0.41
1:A:1662:GLU:HB2	1:A:1666:MET:HE2	2.01	0.41
1:A:118:PHE:O	1:A:122:ILE:HG13	2.19	0.41
1:A:846:MET:HE2	1:A:846:MET:HB3	1.99	0.41
1:A:269:CYS:O	1:A:369:ALA:HA	2.21	0.41
1:A:335:LYS:HE2	1:A:335:LYS:HB2	1.83	0.41
1:A:1398:GLN:OE1	1:A:1399:PRO:HD2	2.21	0.41
1:A:110:ASP:O	1:A:114:ILE:HG12	2.21	0.41
1:A:99:TYR:CE1	1:A:101:PRO:HG3	2.56	0.41
1:A:351:PHE:O	1:A:355:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:LEU:HD23	1:A:1247:LEU:HA	1.83	0.41
1:A:1360:LYS:NZ	1:A:1689:ARG:HA	2.35	0.41
1:A:70:ASN:HA	1:A:73:ILE:HG12	2.02	0.40
1:A:109:SER:O	1:A:113:LYS:HG3	2.21	0.40
1:A:1276:LEU:O	1:A:1279:THR:OG1	2.26	0.40
5:A:2310:Y01:HAS2	5:A:2310:Y01:HAE1	1.93	0.40
1:A:1183:ASN:HD22	1:A:1215:PHE:HE2	1.69	0.40
1:A:189:ILE:HD13	1:A:199:VAL:HG21	2.02	0.40
1:A:1271:LEU:HD23	1:A:1271:LEU:HA	1.85	0.40
1:A:1305:PRO:HG2	1:A:1432:GLU:CG	2.40	0.40
1:A:1421:PHE:O	1:A:1425:MET:HG3	2.22	0.40
1:A:1596:LEU:HA	1:A:1599:LEU:HD23	2.04	0.40
1:A:1250:VAL:HG11	1:A:1277:LEU:CB	2.52	0.40
1:A:1279:THR:CG2	1:A:1639:GLU:HG3	2.51	0.40
1:A:1321:GLY:O	1:A:1325:VAL:HG23	2.22	0.40
1:A:1370:LEU:HD23	1:A:1370:LEU:HA	1.77	0.40
1:A:1441:GLN:OE1	1:A:1445:GLU:HB2	2.20	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	1128/2223 (51%)	1053 (93%)	75 (7%)	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	1006/1879 (54%)	1005 (100%)	1 (0%)	93 98

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

Mol	Chain	Res	Type
1	A	1379	LYS

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

Mol	Chain	Res	Type
1	A	332	ASN
1	A	653	ASN
1	A	816	GLN
1	A	1500	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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$
5	Y01	A	2308	-	34,34,38	0.73	1 (2%)	52,52,57	1.64	9 (17%)
5	Y01	A	2312	-	38,38,38	0.71	0	57,57,57	1.72	13 (22%)
6	NAG	A	2311	1	14,14,15	0.38	0	17,19,21	1.29	1 (5%)
5	Y01	A	2316	-	38,38,38	0.62	0	57,57,57	1.69	12 (21%)
2	7TB	A	2301	-	36,36,36	1.64	8 (22%)	46,46,46	1.29	5 (10%)
5	Y01	A	2310	-	38,38,38	0.75	1 (2%)	57,57,57	1.62	12 (21%)
3	3PE	A	2303	-	8,8,50	1.47	0	7,7,55	0.76	0
3	3PE	A	2315	-	11,11,50	1.51	0	10,10,55	0.85	0
6	NAG	A	2313	1	14,14,15	0.27	0	17,19,21	0.50	0
3	3PE	A	2302	-	32,32,50	2.36	11 (34%)	36,37,55	1.27	2 (5%)
3	3PE	A	2305	-	10,10,50	1.50	0	9,9,55	0.85	0
5	Y01	A	2314	1	32,32,38	0.81	2 (6%)	49,49,57	1.63	12 (24%)
3	3PE	A	2307	-	11,11,50	1.51	0	10,10,55	0.84	0
5	Y01	A	2309	-	34,34,38	0.78	1 (2%)	52,52,57	1.72	10 (19%)
3	3PE	A	2306	-	11,11,50	1.50	0	10,10,55	0.89	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	Y01	A	2308	-	-	6/14/72/77	0/4/4/4
5	Y01	A	2312	-	-	13/19/77/77	0/4/4/4
6	NAG	A	2311	1	-	5/6/23/26	0/1/1/1
5	Y01	A	2316	-	-	11/19/77/77	0/4/4/4
2	7TB	A	2301	-	-	10/34/34/34	0/2/2/2
5	Y01	A	2310	-	-	13/19/77/77	0/4/4/4
3	3PE	A	2303	-	-	0/6/6/54	-
3	3PE	A	2315	-	-	4/9/9/54	-
6	NAG	A	2313	1	-	3/6/23/26	0/1/1/1
3	3PE	A	2302	-	-	20/34/34/54	-
3	3PE	A	2305	-	-	3/8/8/54	-
5	Y01	A	2314	1	-	8/12/70/77	0/4/4/4
3	3PE	A	2307	-	-	4/9/9/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	A	2309	-	-	11/14/72/77	0/4/4/4
3	3PE	A	2306	-	-	4/9/9/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2301	7TB	C32-N07	5.32	1.49	1.35
3	A	2302	3PE	P-O13	4.76	1.73	1.54
3	A	2302	3PE	O31-C31	4.71	1.47	1.33
3	A	2302	3PE	O21-C21	4.33	1.46	1.34
3	A	2302	3PE	P-O11	4.13	1.73	1.60
2	A	2301	7TB	O02-C18	3.56	1.42	1.33
3	A	2302	3PE	C22-C21	3.40	1.60	1.50
3	A	2302	3PE	C1-C2	3.32	1.60	1.50
3	A	2302	3PE	C32-C31	3.28	1.60	1.50
2	A	2301	7TB	C31-C32	3.26	1.56	1.50
2	A	2301	7TB	C28-N07	3.25	1.48	1.41
3	A	2302	3PE	C3-C2	3.10	1.60	1.50
5	A	2310	Y01	CBH-CBF	-2.59	1.51	1.56
3	A	2302	3PE	P-O14	2.52	1.58	1.50
5	A	2309	Y01	CBH-CBF	-2.46	1.51	1.56
2	A	2301	7TB	O05-C32	-2.46	1.18	1.23
5	A	2308	Y01	CBH-CBF	-2.33	1.52	1.56
3	A	2302	3PE	C23-C22	2.27	1.60	1.52
3	A	2302	3PE	C33-C32	2.20	1.60	1.52
2	A	2301	7TB	C22-C18	2.18	1.55	1.50
5	A	2314	Y01	OAW-CAY	-2.15	1.34	1.42
5	A	2314	Y01	CBH-CBF	-2.13	1.52	1.56
2	A	2301	7TB	C08-C12	2.12	1.58	1.51
2	A	2301	7TB	O03-C27	2.07	1.41	1.37

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2312	Y01	CBI-CBE-CBB	-5.40	111.03	119.49
5	A	2309	Y01	OAW-CAY-CAM	5.01	120.30	111.09
5	A	2309	Y01	CBI-CBE-CBB	-4.97	111.71	119.49
5	A	2308	Y01	OAW-CAY-CAM	4.86	120.03	111.09
5	A	2316	Y01	CBI-CBE-CBB	-4.75	112.05	119.49
5	A	2310	Y01	CBI-CBE-CBB	-4.65	112.20	119.49
6	A	2311	NAG	C2-N2-C7	4.41	129.19	122.90
2	A	2301	7TB	O02-C18-C22	4.28	119.60	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2301	7TB	C12-C08-N06	-4.27	110.11	116.15
5	A	2308	Y01	CBI-CBE-CBB	-4.19	112.93	119.49
3	A	2302	3PE	O21-C21-C22	4.16	120.47	111.50
5	A	2316	Y01	OAW-CAY-CAM	4.06	120.26	111.50
5	A	2316	Y01	CBI-CBG-CBD	-4.04	108.39	114.38
5	A	2312	Y01	CAQ-CBG-CBI	-3.83	99.23	103.84
5	A	2310	Y01	OAW-CAY-CAM	3.81	119.71	111.50
5	A	2314	Y01	CBI-CBE-CBB	-3.74	113.62	119.49
5	A	2309	Y01	CBI-CBG-CBD	-3.73	108.85	114.38
5	A	2312	Y01	OAW-CAY-CAM	3.50	119.03	111.50
5	A	2316	Y01	CBD-CAK-CAI	-3.44	107.79	112.73
5	A	2312	Y01	CBI-CBG-CBD	-3.38	109.37	114.38
5	A	2308	Y01	CBI-CBG-CBD	-3.27	109.53	114.38
5	A	2316	Y01	CBF-CBH-CAZ	3.22	114.70	109.65
5	A	2309	Y01	CBF-CBH-CAZ	3.19	114.66	109.65
5	A	2314	Y01	CBI-CBG-CBD	-3.19	109.66	114.38
5	A	2314	Y01	CAD-CBH-CBF	-3.17	107.90	111.68
5	A	2310	Y01	CAQ-CBG-CBI	-2.96	100.28	103.84
5	A	2314	Y01	CAQ-CBG-CBI	-2.91	100.33	103.84
5	A	2312	Y01	CAQ-CBG-CBD	-2.89	114.32	119.08
3	A	2302	3PE	O31-C31-C32	2.86	120.88	111.91
5	A	2308	Y01	CBF-CBD-CBG	-2.82	105.32	109.09
5	A	2309	Y01	CAD-CBH-CBF	-2.81	108.33	111.68
5	A	2308	Y01	CBF-CBH-CAZ	2.80	114.05	109.65
5	A	2314	Y01	CBH-CBF-CBD	-2.78	108.56	112.73
5	A	2310	Y01	CAD-CBH-CBF	-2.76	108.39	111.68
5	A	2309	Y01	CAS-CAU-CBI	-2.71	108.14	112.78
5	A	2312	Y01	CBD-CAK-CAI	-2.70	108.85	112.73
5	A	2314	Y01	CBD-CAK-CAI	-2.70	108.86	112.73
5	A	2316	Y01	CAV-CAZ-CAI	-2.65	116.79	120.61
5	A	2314	Y01	CAT-CBH-CBF	2.64	112.42	108.73
5	A	2309	Y01	CAC-CBB-CBE	-2.54	109.03	112.92
5	A	2310	Y01	CAC-CBB-CBE	-2.54	109.03	112.92
5	A	2312	Y01	CAC-CBB-CBE	-2.52	109.07	112.92
5	A	2309	Y01	CBF-CBD-CBG	-2.51	105.74	109.09
5	A	2310	Y01	CAS-CAU-CBI	-2.48	108.52	112.78
5	A	2316	Y01	CAQ-CBG-CBI	-2.46	100.88	103.84
2	A	2301	7TB	O03-C27-C33	-2.45	118.67	123.97
5	A	2308	Y01	CAD-CBH-CBF	-2.43	108.78	111.68
5	A	2312	Y01	CBF-CBH-CAZ	2.42	113.45	109.65
5	A	2312	Y01	CAK-CBD-CBG	-2.42	107.40	110.91
5	A	2310	Y01	CAM-CAL-CAX	-2.42	108.41	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2314	Y01	CAQ-CBG-CBD	-2.41	115.11	119.08
5	A	2310	Y01	CBI-CBG-CBD	-2.37	110.87	114.38
5	A	2309	Y01	CAQ-CBG-CBD	-2.35	115.20	119.08
5	A	2310	Y01	CBC-CAV-CAZ	-2.35	107.86	111.52
5	A	2308	Y01	CAS-CBF-CBD	-2.34	108.38	111.75
5	A	2308	Y01	CAQ-CBG-CBI	-2.31	101.06	103.84
5	A	2314	Y01	CAP-CAQ-CBG	-2.28	100.62	105.13
5	A	2312	Y01	CAV-CAZ-CAI	-2.28	117.33	120.61
2	A	2301	7TB	C27-C31-C32	-2.24	122.07	126.16
5	A	2312	Y01	CAS-CAU-CBI	-2.23	108.95	112.78
5	A	2312	Y01	CAD-CBH-CBF	-2.22	109.04	111.68
5	A	2314	Y01	CAS-CAU-CBI	-2.17	109.05	112.78
2	A	2301	7TB	O03-C27-C31	2.15	121.97	117.02
5	A	2316	Y01	CBF-CBD-CBG	-2.14	106.22	109.09
5	A	2316	Y01	CAC-CBB-CBE	-2.14	109.64	112.92
5	A	2316	Y01	CBG-CBI-CBE	2.13	102.60	100.07
5	A	2316	Y01	CBC-CAV-CAZ	-2.12	108.23	111.52
5	A	2309	Y01	CAQ-CBG-CBI	-2.10	101.31	103.84
5	A	2310	Y01	CAK-CBD-CBG	-2.09	107.87	110.91
5	A	2314	Y01	CAT-CAR-CBC	2.08	113.87	110.33
5	A	2308	Y01	CBD-CAK-CAI	-2.06	109.77	112.73
5	A	2310	Y01	CBF-CBH-CAZ	2.04	112.85	109.65
5	A	2314	Y01	CBG-CBI-CBE	2.04	102.49	100.07
5	A	2310	Y01	CAS-CBF-CBH	-2.02	110.42	113.08
5	A	2316	Y01	CAS-CAU-CBI	-2.01	109.33	112.78
5	A	2312	Y01	CAT-CBH-CBF	2.00	111.52	108.73

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2302	3PE	C1-O11-P-O12
3	A	2302	3PE	C1-O11-P-O13
5	A	2309	Y01	CAC-CBB-CBE-CBI
5	A	2309	Y01	OAG-CAY-OAW-CBC
5	A	2309	Y01	CAM-CAY-OAW-CBC
5	A	2310	Y01	CAM-CAY-OAW-CBC
5	A	2312	Y01	CAO-CBB-CBE-CAP
5	A	2312	Y01	CAC-CBB-CBE-CBI
5	A	2308	Y01	CAM-CAY-OAW-CBC
2	A	2301	7TB	C22-C18-O02-C12
2	A	2301	7TB	O04-C18-O02-C12

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Mol	Chain	Res	Type	Atoms
5	A	2316	Y01	CAJ-CAO-CBB-CAC
5	A	2312	Y01	CAC-CBB-CBE-CAP
5	A	2310	Y01	CAC-CBB-CBE-CBI
5	A	2312	Y01	CAO-CBB-CBE-CBI
5	A	2310	Y01	OAG-CAY-OAW-CBC
5	A	2312	Y01	CAJ-CAO-CBB-CAC
5	A	2309	Y01	CAC-CBB-CBE-CAP
5	A	2309	Y01	CAO-CBB-CBE-CBI
5	A	2310	Y01	CAO-CBB-CBE-CBI
5	A	2308	Y01	OAG-CAY-OAW-CBC
6	A	2313	NAG	C4-C5-C6-O6
5	A	2309	Y01	CAO-CBB-CBE-CAP
5	A	2314	Y01	CAJ-CAO-CBB-CAC
6	A	2313	NAG	O5-C5-C6-O6
5	A	2316	Y01	CAO-CBB-CBE-CBI
5	A	2314	Y01	CAJ-CAO-CBB-CBE
6	A	2311	NAG	C4-C5-C6-O6
6	A	2311	NAG	C8-C7-N2-C2
6	A	2311	NAG	O7-C7-N2-C2
5	A	2312	Y01	CAO-CAJ-CAN-CBA
5	A	2309	Y01	CAJ-CAO-CBB-CAC
5	A	2316	Y01	CAC-CBB-CBE-CBI
5	A	2310	Y01	CAN-CAJ-CAO-CBB
5	A	2309	Y01	CAJ-CAO-CBB-CBE
5	A	2312	Y01	CAJ-CAO-CBB-CBE
5	A	2316	Y01	CAN-CAJ-CAO-CBB
2	A	2301	7TB	C29-C28-N07-C32
2	A	2301	7TB	C30-C28-N07-C32
5	A	2310	Y01	CAO-CAJ-CAN-CBA
5	A	2316	Y01	CAJ-CAO-CBB-CBE
5	A	2310	Y01	CAC-CBB-CBE-CAP
5	A	2312	Y01	CAX-CAL-CAM-CAY
5	A	2312	Y01	CAN-CAJ-CAO-CBB
5	A	2314	Y01	CAC-CBB-CBE-CBI
5	A	2314	Y01	CAO-CBB-CBE-CBI
5	A	2309	Y01	CAJ-CAN-CBA-CAB
3	A	2302	3PE	C33-C34-C35-C36
5	A	2309	Y01	CAJ-CAN-CBA-CAA
6	A	2311	NAG	O5-C5-C6-O6
3	A	2302	3PE	C32-C33-C34-C35
3	A	2302	3PE	C23-C24-C25-C26
3	A	2302	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	A	2301	7TB	C17-C15-C16-C19
3	A	2302	3PE	C27-C28-C29-C2A
5	A	2310	Y01	CAX-CAL-CAM-CAY
5	A	2309	Y01	CAN-CAJ-CAO-CBB
3	A	2306	3PE	C37-C38-C39-C3A
3	A	2302	3PE	C22-C23-C24-C25
2	A	2301	7TB	C27-C31-C32-O05
3	A	2305	3PE	C33-C34-C35-C36
2	A	2301	7TB	C15-C17-C20-C23
2	A	2301	7TB	C27-C31-C32-N07
3	A	2302	3PE	O22-C21-O21-C2
3	A	2302	3PE	C21-C22-C23-C24
5	A	2314	Y01	CAO-CAJ-CAN-CBA
5	A	2314	Y01	CAV-CBC-OAW-CAY
5	A	2308	Y01	CAC-CBB-CBE-CBI
3	A	2302	3PE	C1-O11-P-O14
3	A	2302	3PE	C25-C26-C27-C28
5	A	2314	Y01	CAC-CBB-CBE-CAP
5	A	2316	Y01	CAC-CBB-CBE-CAP
5	A	2316	Y01	CAO-CAJ-CAN-CBA
5	A	2310	Y01	CAO-CBB-CBE-CAP
5	A	2316	Y01	CAO-CBB-CBE-CAP
3	A	2302	3PE	C31-C32-C33-C34
3	A	2315	3PE	C39-C3A-C3B-C3C
5	A	2314	Y01	CAO-CBB-CBE-CAP
3	A	2307	3PE	C3C-C3D-C3E-C3F
2	A	2301	7TB	C20-C23-O03-C27
3	A	2302	3PE	C28-C29-C2A-C2B
3	A	2307	3PE	C39-C3A-C3B-C3C
3	A	2302	3PE	O11-C1-C2-C3
5	A	2308	Y01	CAO-CBB-CBE-CBI
3	A	2302	3PE	O11-C1-C2-O21
5	A	2312	Y01	CAV-CBC-OAW-CAY
3	A	2315	3PE	C35-C36-C37-C38
3	A	2305	3PE	C37-C38-C39-C3A
5	A	2308	Y01	CAC-CBB-CBE-CAP
3	A	2307	3PE	C3A-C3B-C3C-C3D
6	A	2313	NAG	C3-C2-N2-C7
5	A	2310	Y01	CAM-CAL-CAX-OAF
3	A	2306	3PE	C39-C3A-C3B-C3C
3	A	2306	3PE	C33-C34-C35-C36
5	A	2316	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
5	A	2312	Y01	OAG-CAY-OAW-CBC
3	A	2315	3PE	C36-C37-C38-C39
5	A	2310	Y01	CAM-CAL-CAX-OAH
3	A	2306	3PE	C38-C39-C3A-C3B
3	A	2307	3PE	C37-C38-C39-C3A
3	A	2302	3PE	O31-C31-C32-C33
5	A	2310	Y01	CAL-CAM-CAY-OAW
5	A	2312	Y01	CAR-CBC-OAW-CAY
3	A	2302	3PE	O21-C21-C22-C23
5	A	2316	Y01	CAL-CAM-CAY-OAW
3	A	2305	3PE	C32-C33-C34-C35
5	A	2312	Y01	CAM-CAY-OAW-CBC
3	A	2302	3PE	O22-C21-C22-C23
6	A	2311	NAG	C3-C2-N2-C7
3	A	2302	3PE	O32-C31-C32-C33
5	A	2310	Y01	CAL-CAM-CAY-OAG
5	A	2316	Y01	CAL-CAM-CAY-OAG
2	A	2301	7TB	N06-C08-C12-O02
5	A	2308	Y01	CAO-CBB-CBE-CAP
3	A	2315	3PE	C34-C35-C36-C37

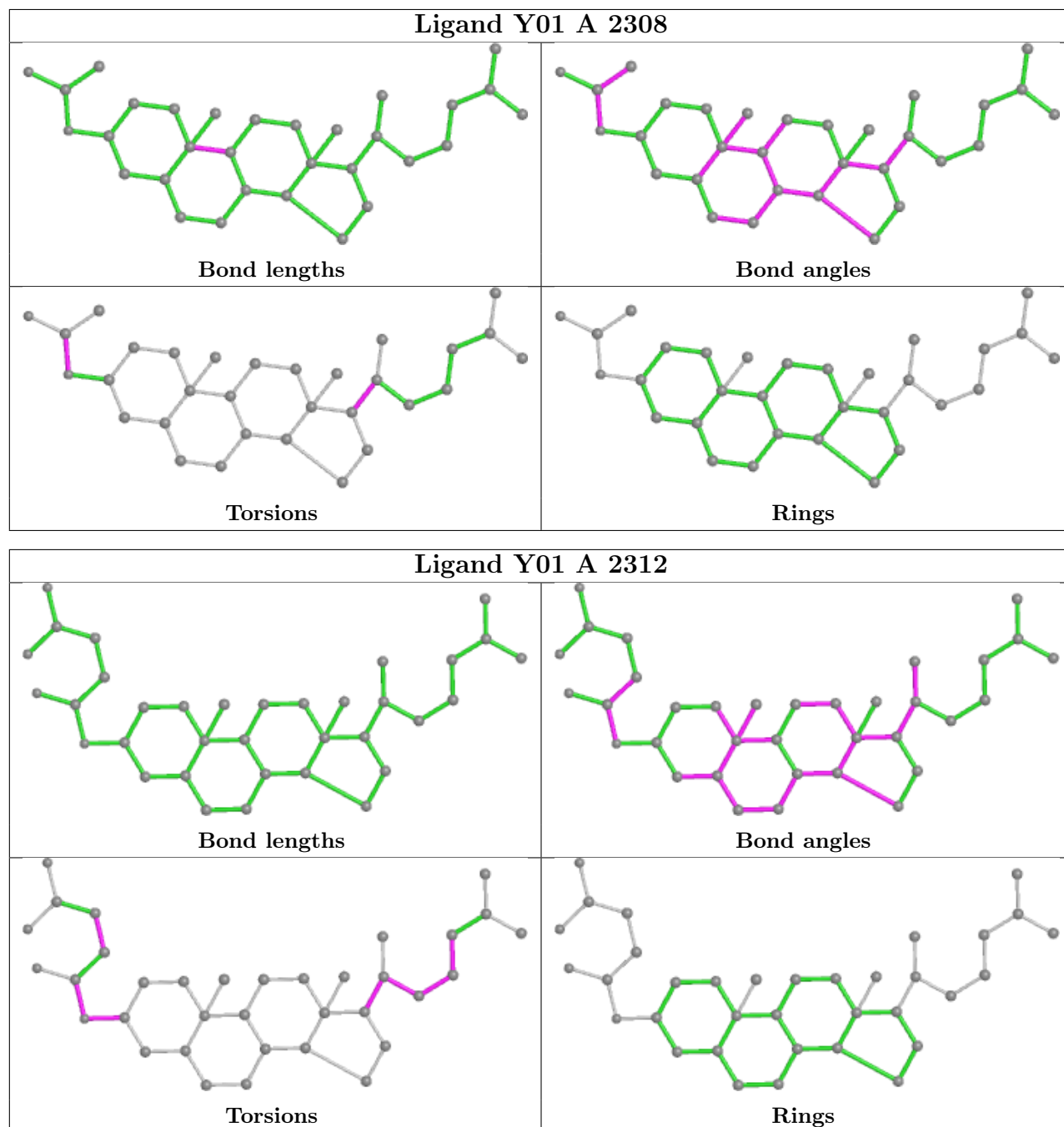
There are no ring outliers.

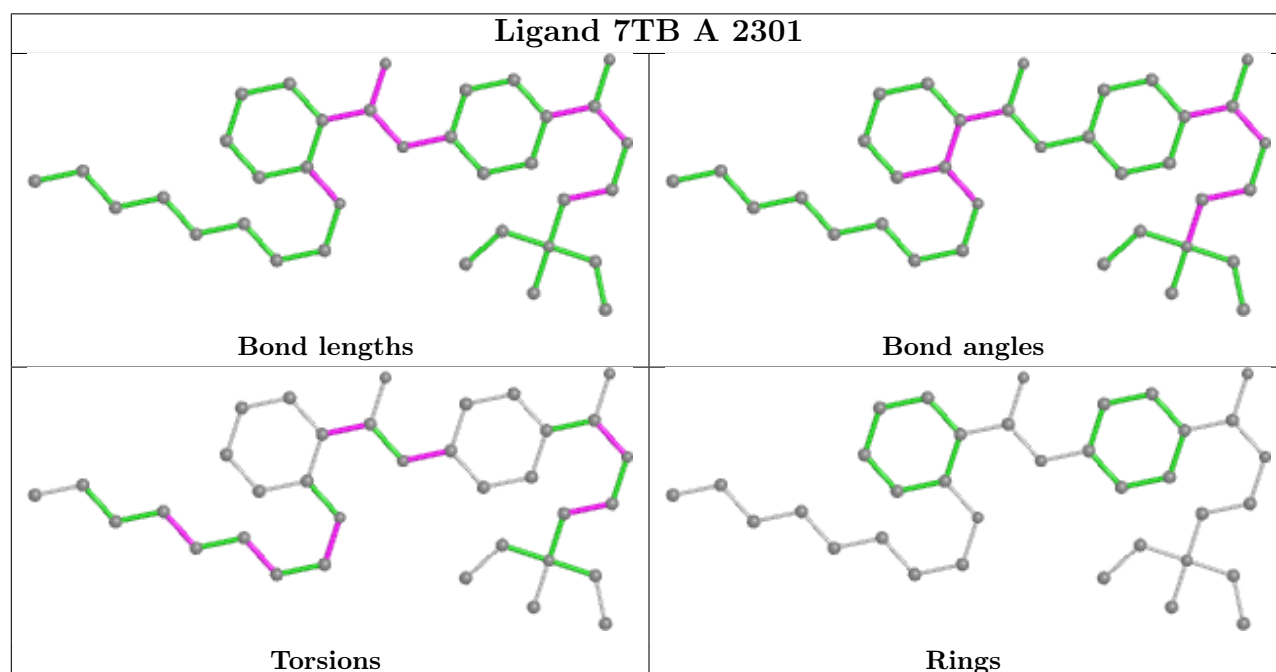
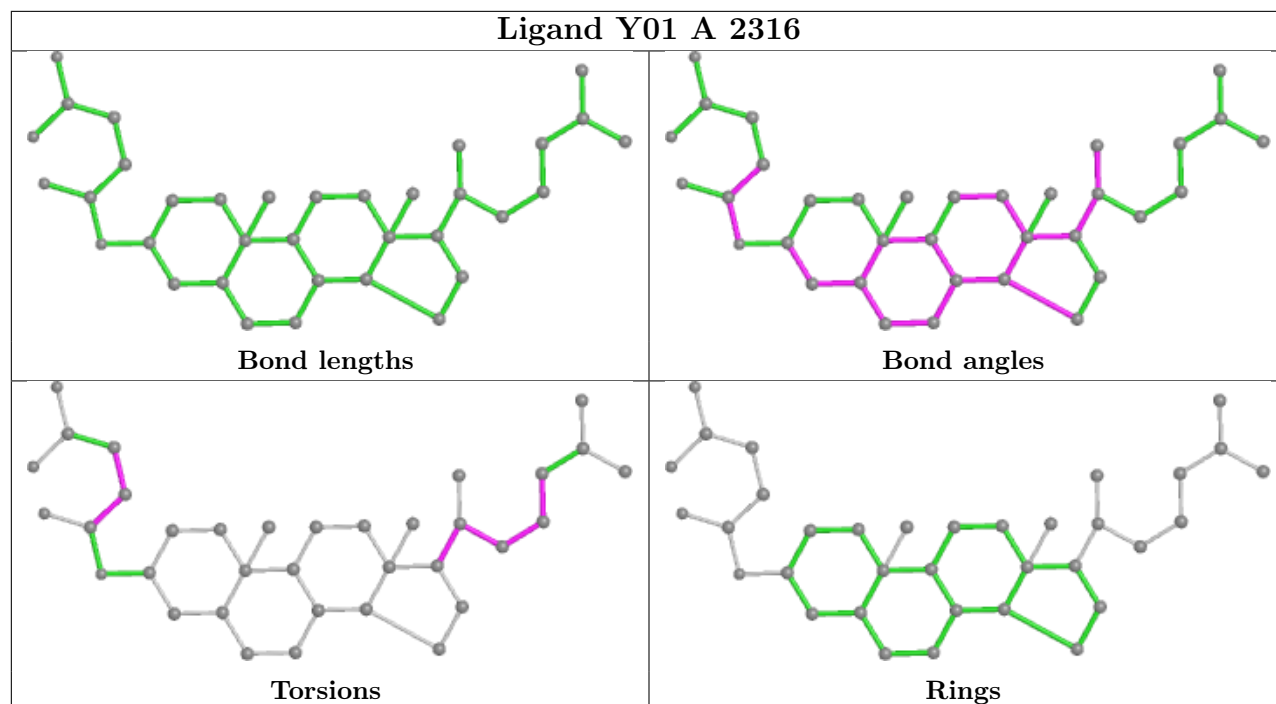
9 monomers are involved in 26 short contacts:

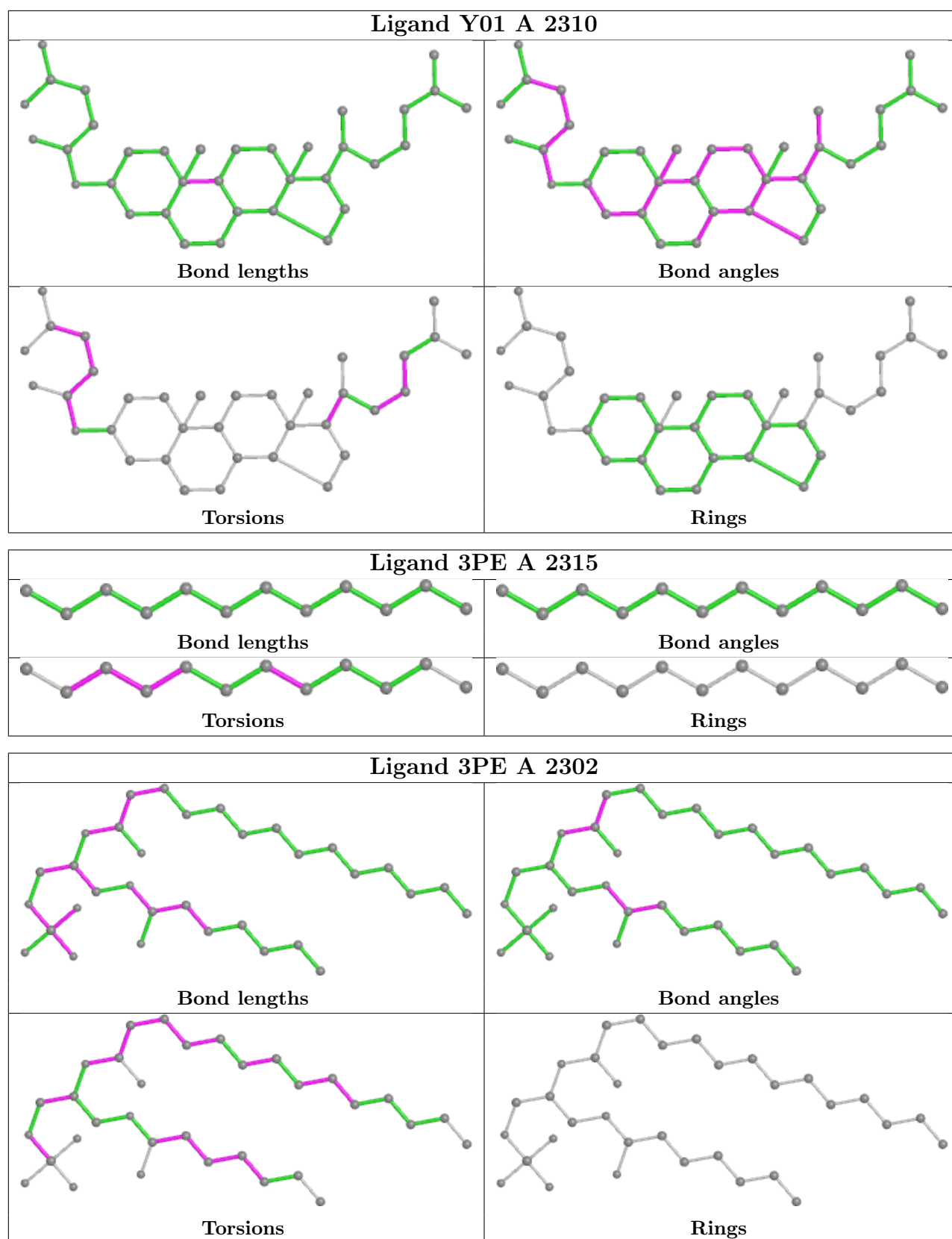
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2308	Y01	3	0
5	A	2312	Y01	3	0
6	A	2311	NAG	1	0
5	A	2316	Y01	6	0
5	A	2310	Y01	3	0
3	A	2315	3PE	1	0
3	A	2302	3PE	1	0
5	A	2314	Y01	7	0
5	A	2309	Y01	2	0

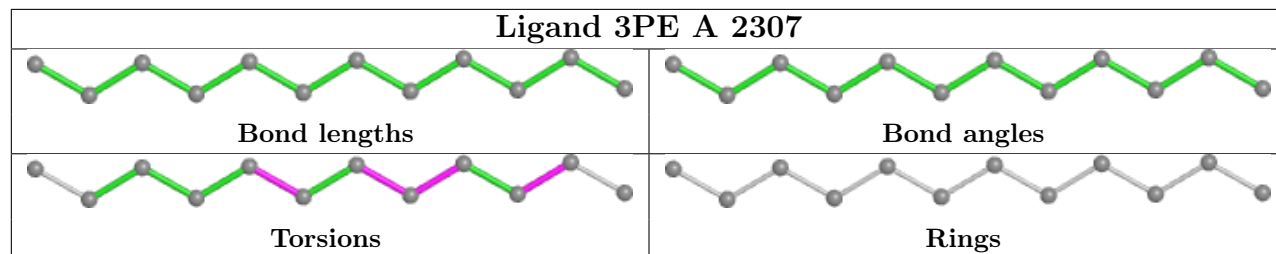
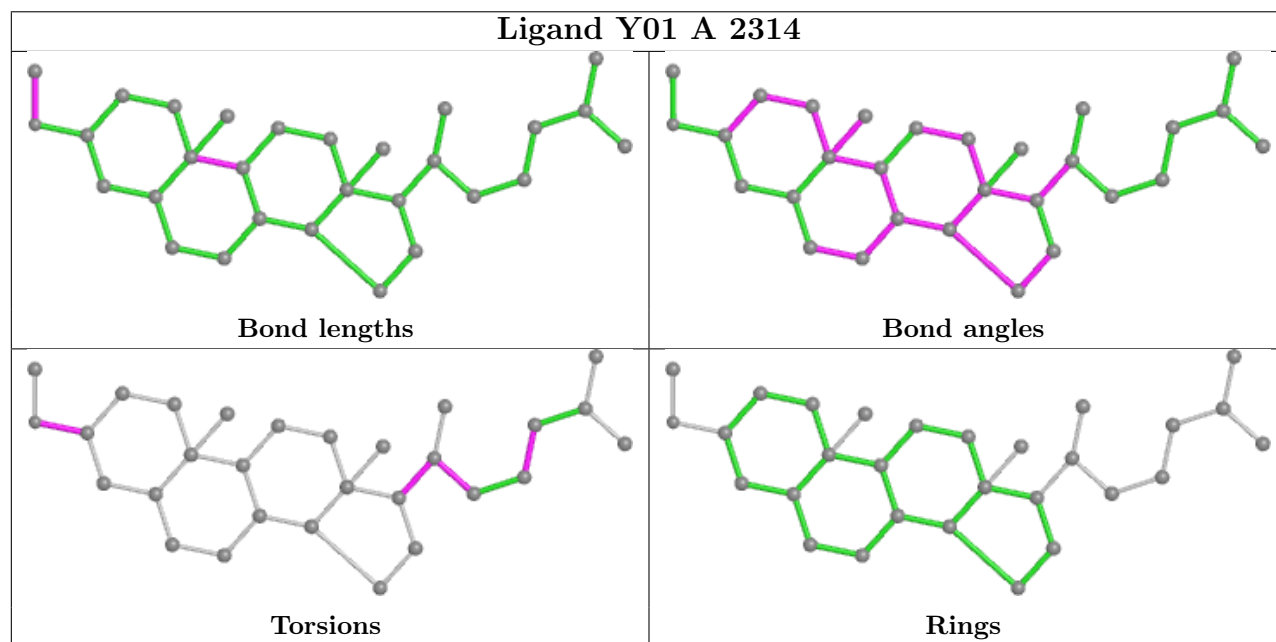
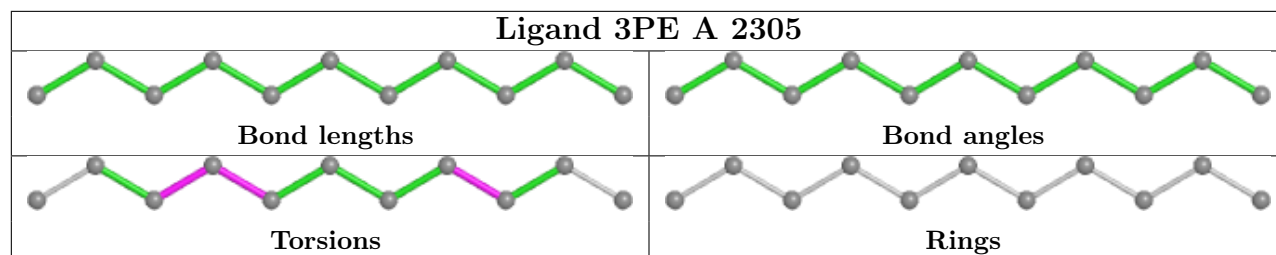
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

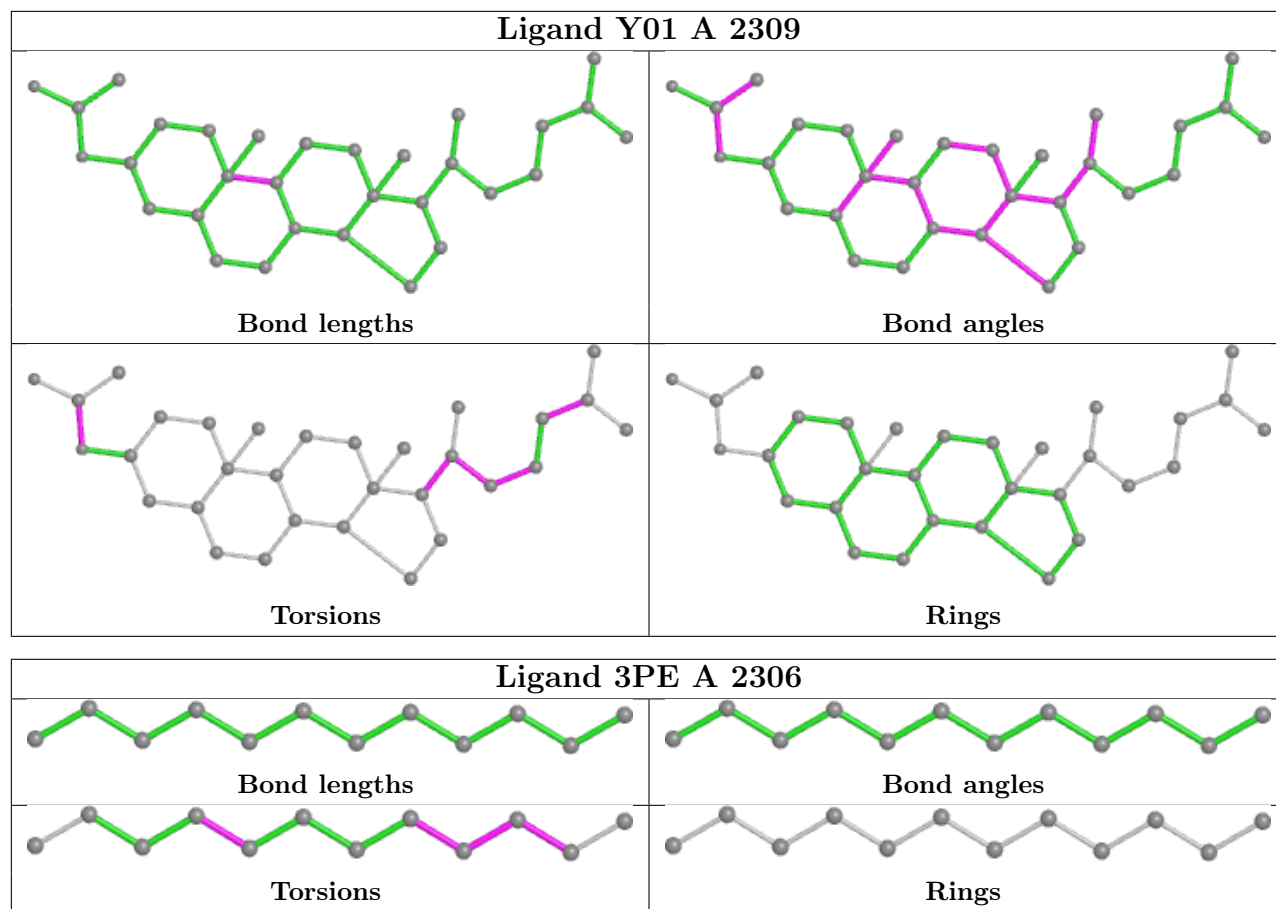
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

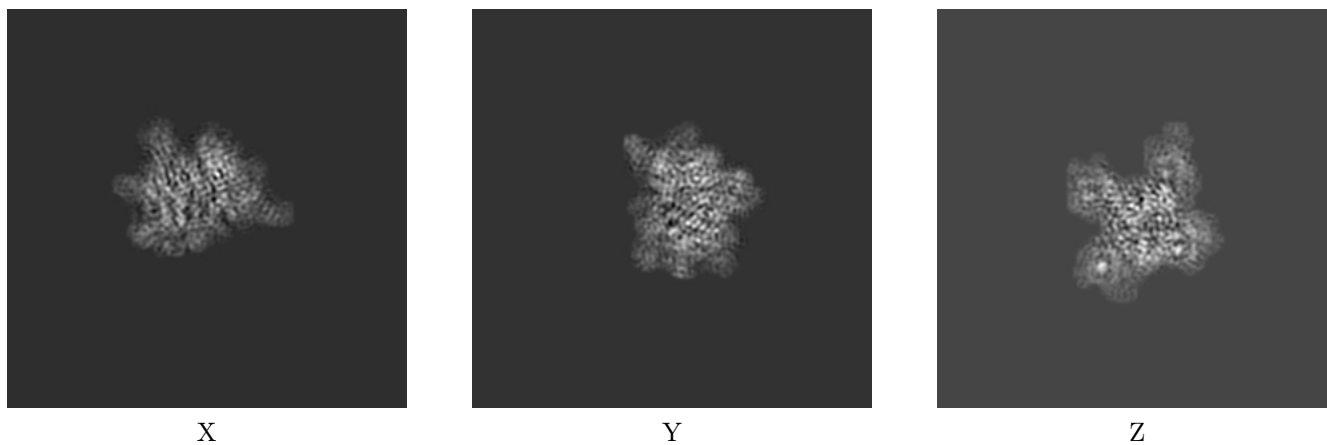
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32586. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

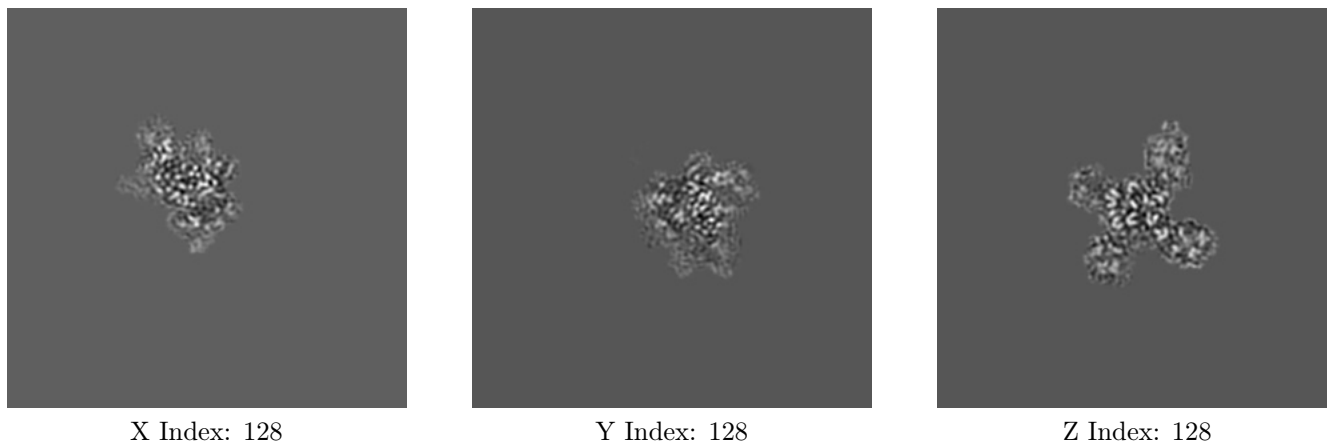
6.1.1 Primary map



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

6.2 Central slices [i](#)

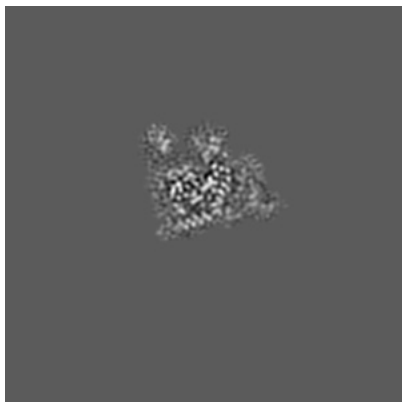
6.2.1 Primary map



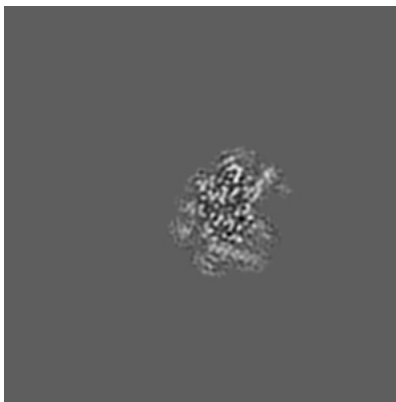
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

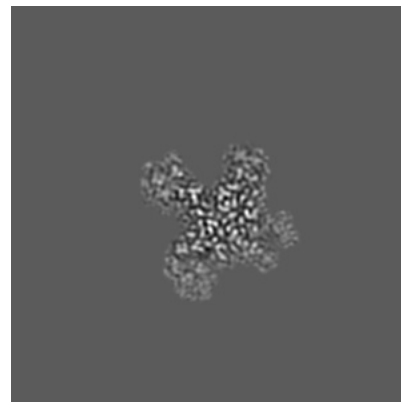
6.3.1 Primary map



X Index: 143



Y Index: 135

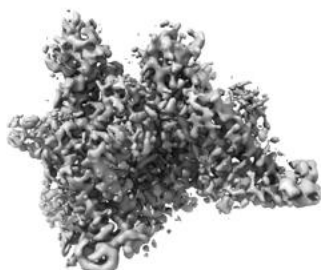


Z Index: 141

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

6.4 Orthogonal surface views [i](#)

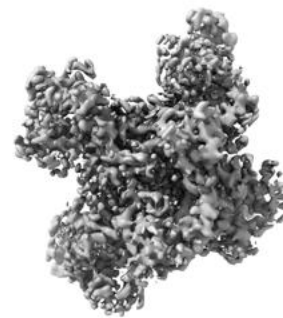
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

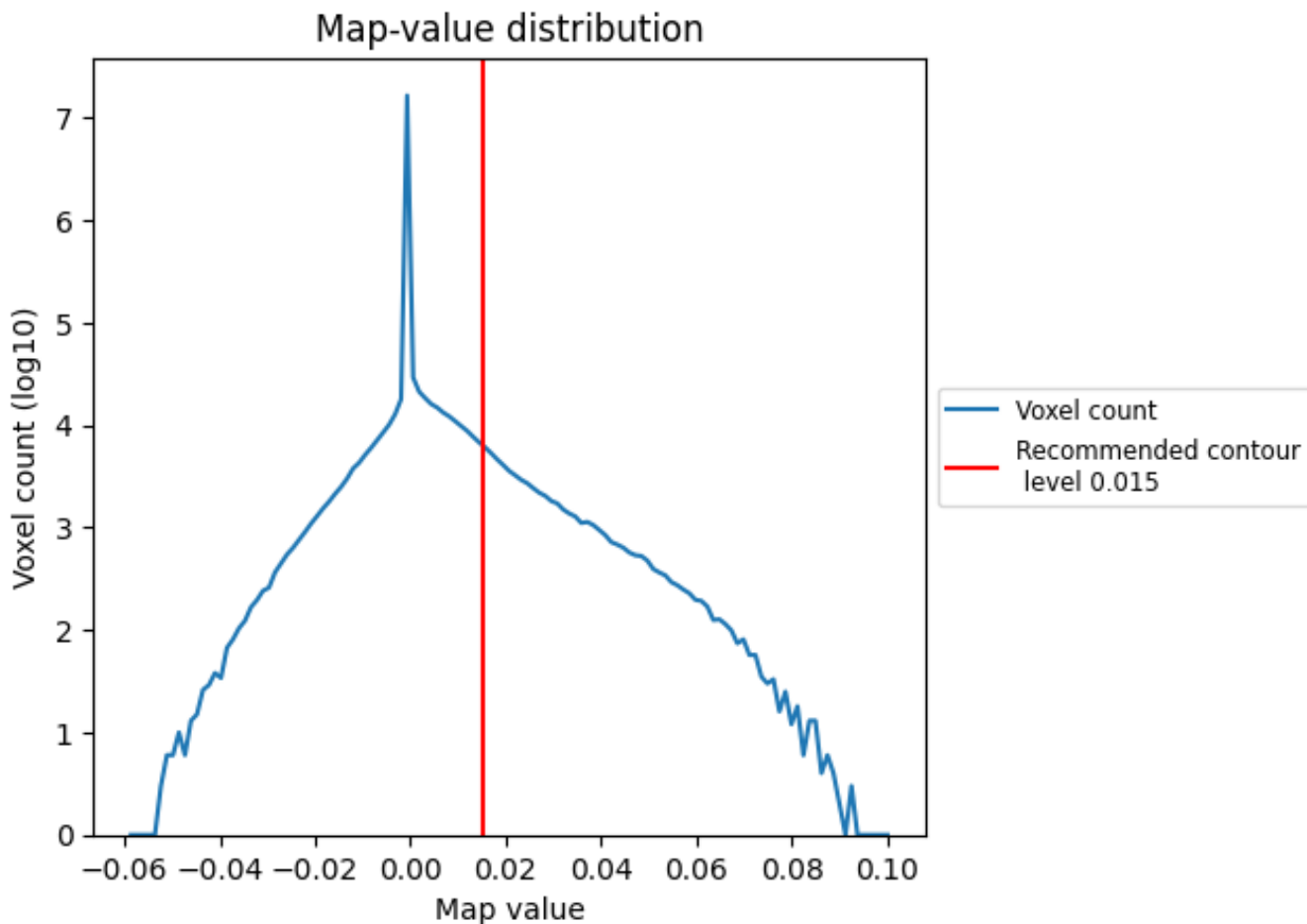
6.5 Mask visualisation

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

7 Map analysis [i](#)

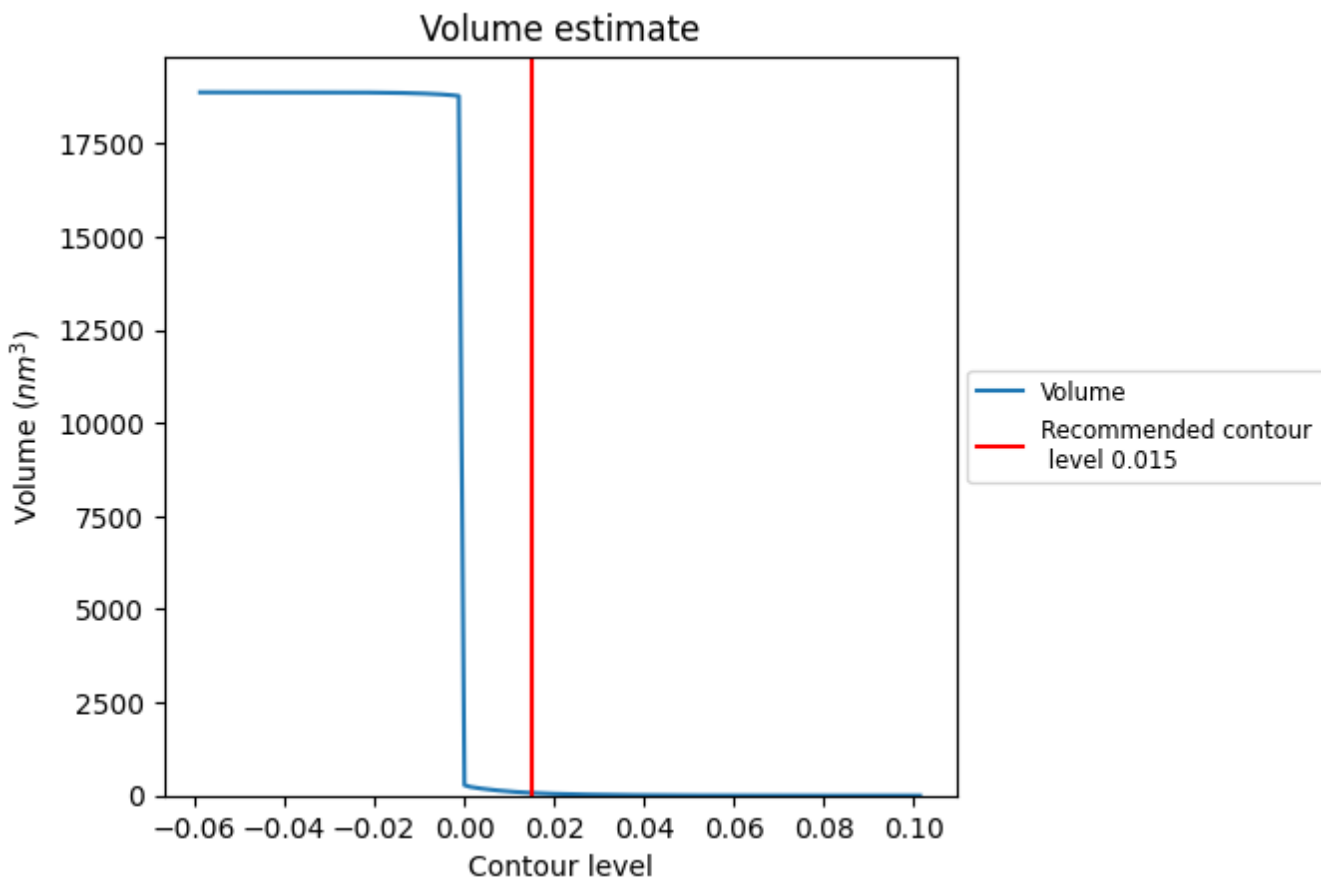
This section contains the results of statistical analysis of the map.

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.

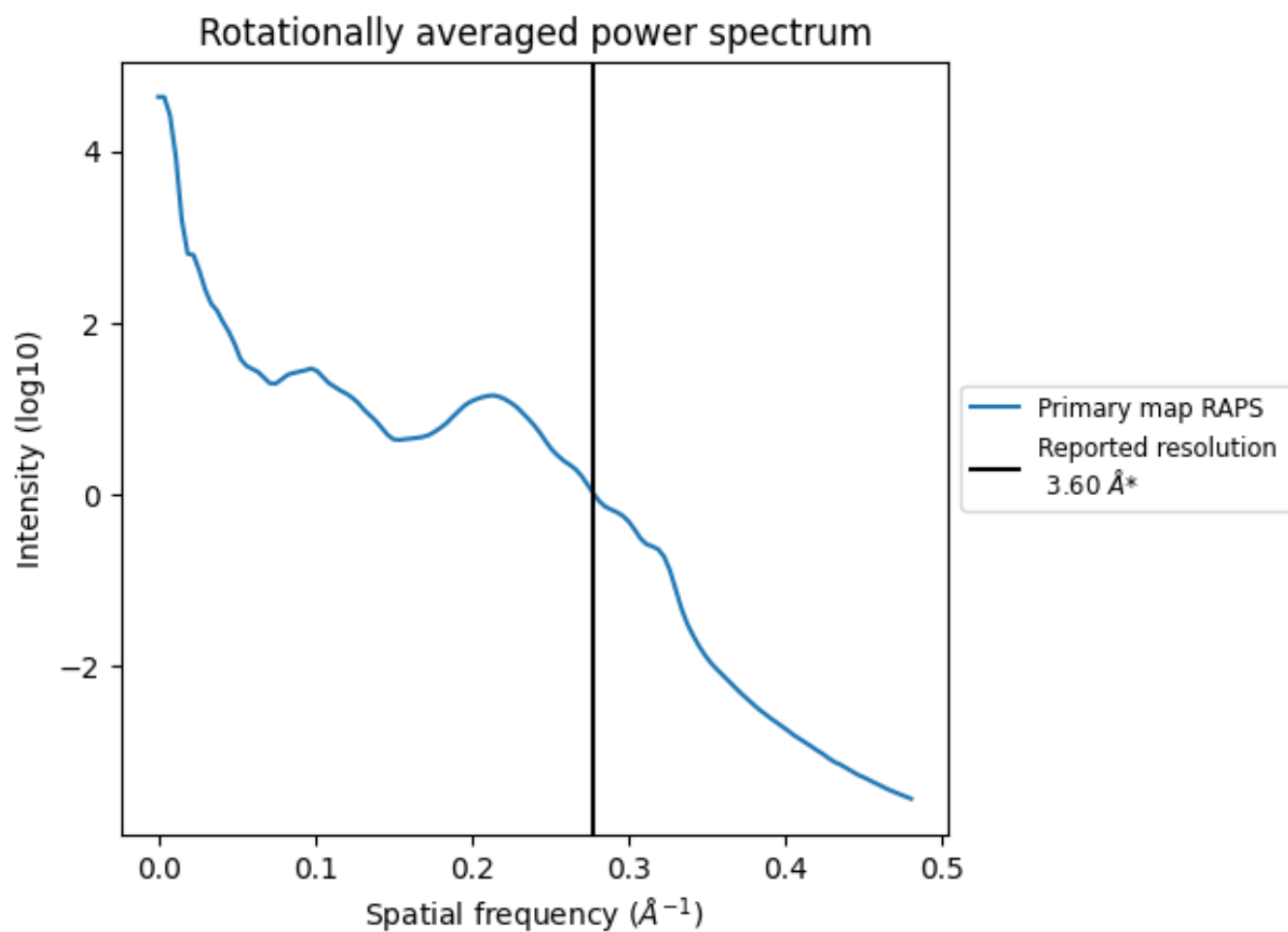
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

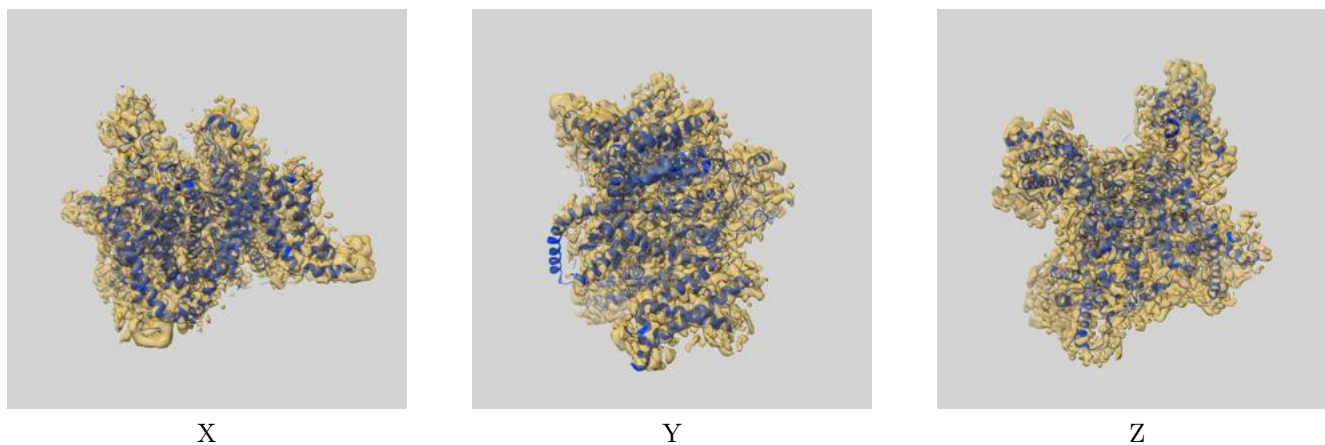
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

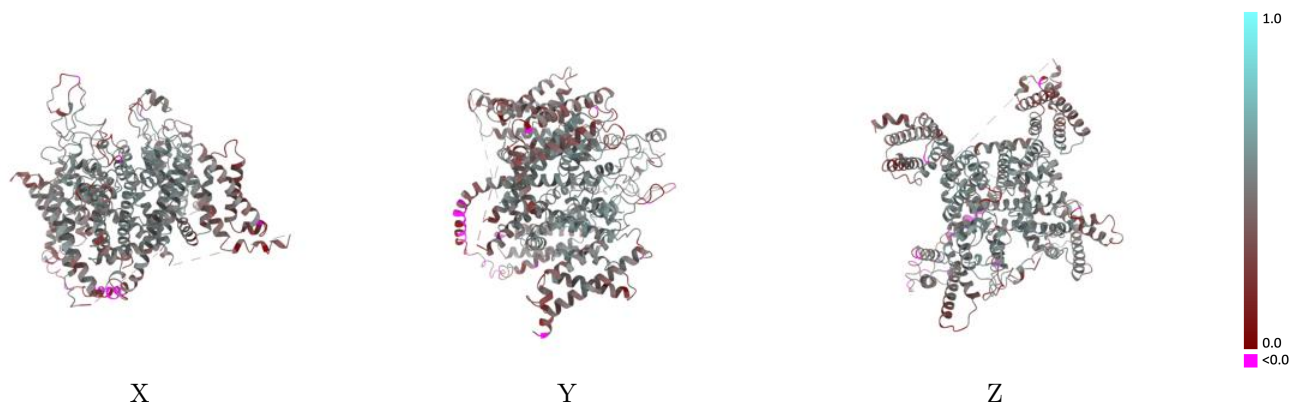
This section contains information regarding the fit between EMDB map EMD-32586 and PDB model 7WLK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



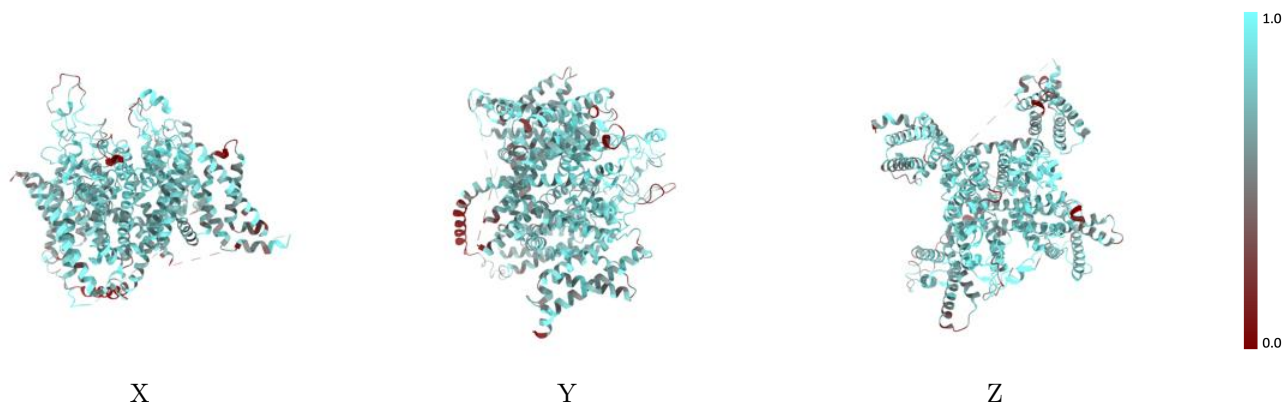
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



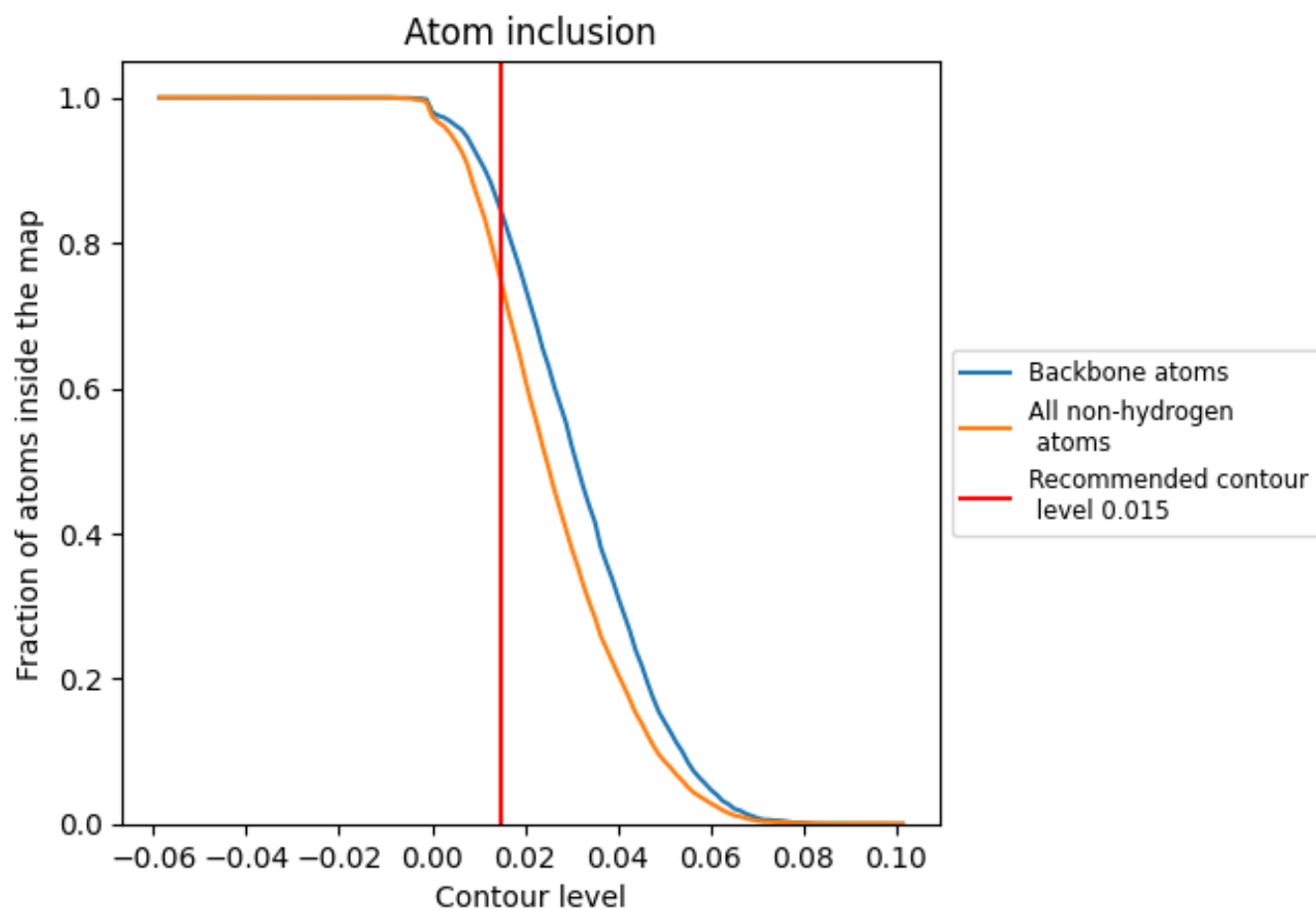
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).





9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7444	 0.4380
A	 0.7444	 0.4380

