



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 12:01 PM EST

PDB ID : 9O8G / pdb\_00009o8g  
EMDB ID : EMD-70226  
Title : Cryo-EM structure of primidone-bound rabbit TRPM3 having 1 resting and 3 activated subunits at 18 degrees Celsius  
Authors : Kumar, S.; Lu, W.; Du, J.  
Deposited on : 2025-04-15  
Resolution : 3.48 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

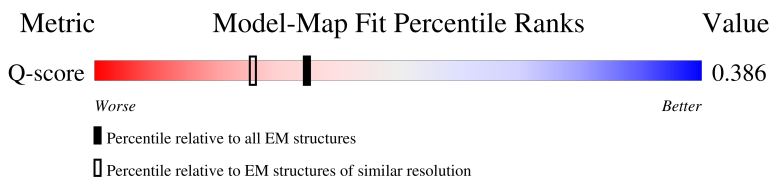
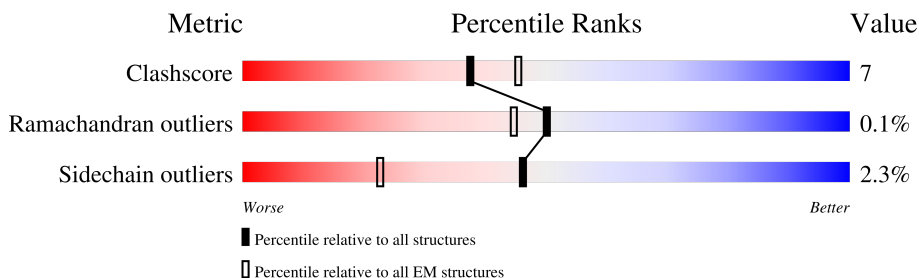
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.47

# 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 3.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13672 ( 2.98 - 3.98 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1306	
1	B	1306	
1	C	1306	
1	D	1306	

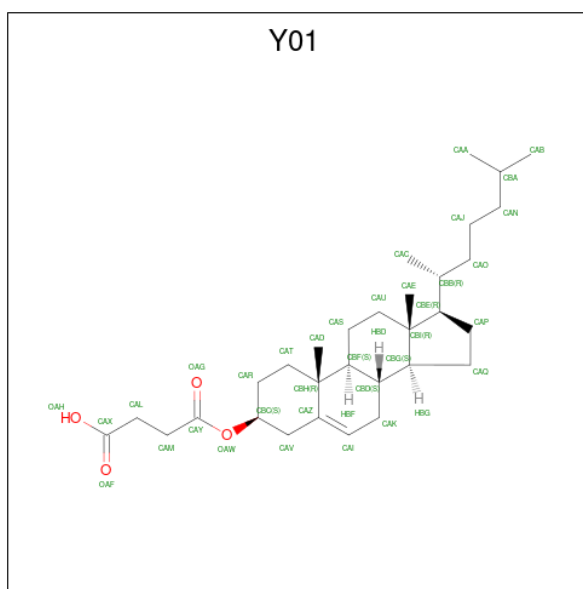
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In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRPM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1052	Total 7807	C 5035	N 1338	O 1377	S 57	1	0
1	D	1045	Total 7787	C 5023	N 1337	O 1370	S 57	2	0
1	B	1042	Total 7773	C 5015	N 1337	O 1364	S 57	2	0
1	C	1061	Total 8019	C 5197	N 1366	O 1397	S 59	1	0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula:  $C_{31}H_{50}O_4$ ).



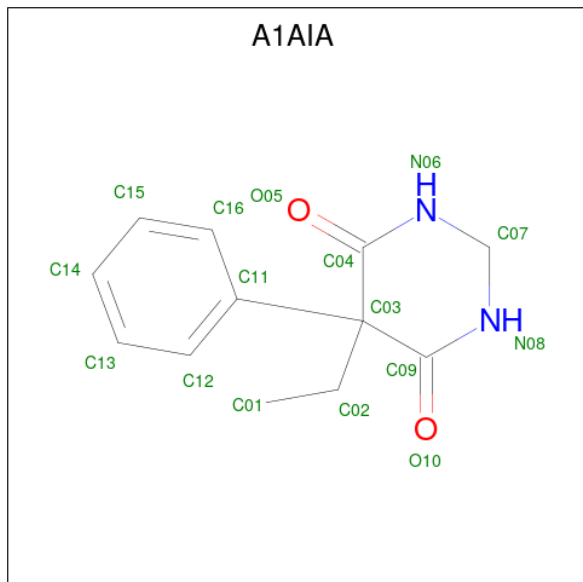
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 35	C 31	O 4	0
2	A	1	Total 35	C 31	O 4	0
2	A	1	Total 35	C 31	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	

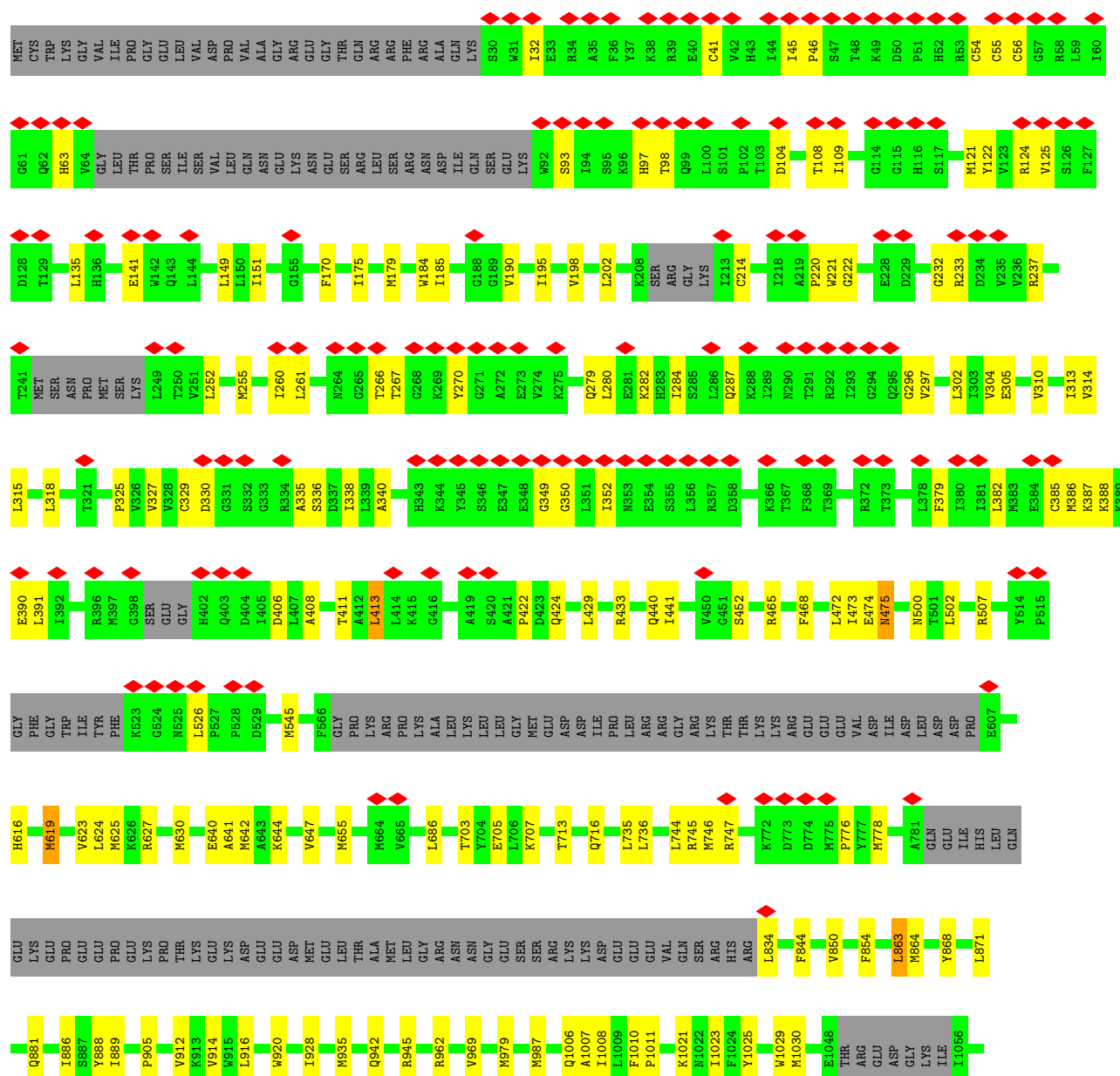
- Molecule 3 is primidone (CCD ID: A1AIA) (formula:  $C_{12}H_{14}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).

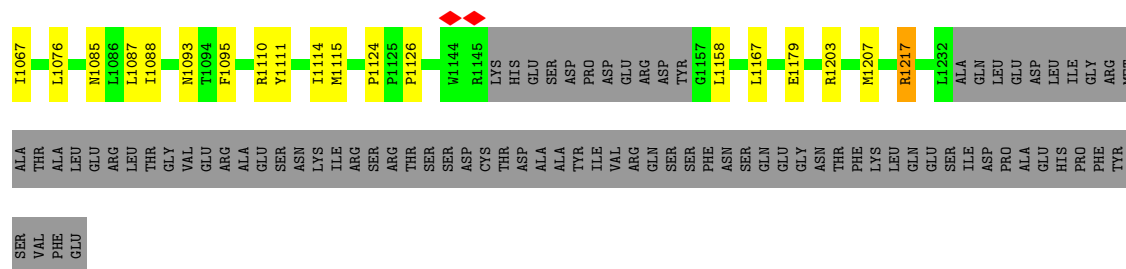


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			16	12	2	2	
3	D	1	Total	C	N	O	0
			16	12	2	2	
3	B	1	Total	C	N	O	0
			16	12	2	2	
3	C	1	Total	C	N	O	0
			16	12	2	2	

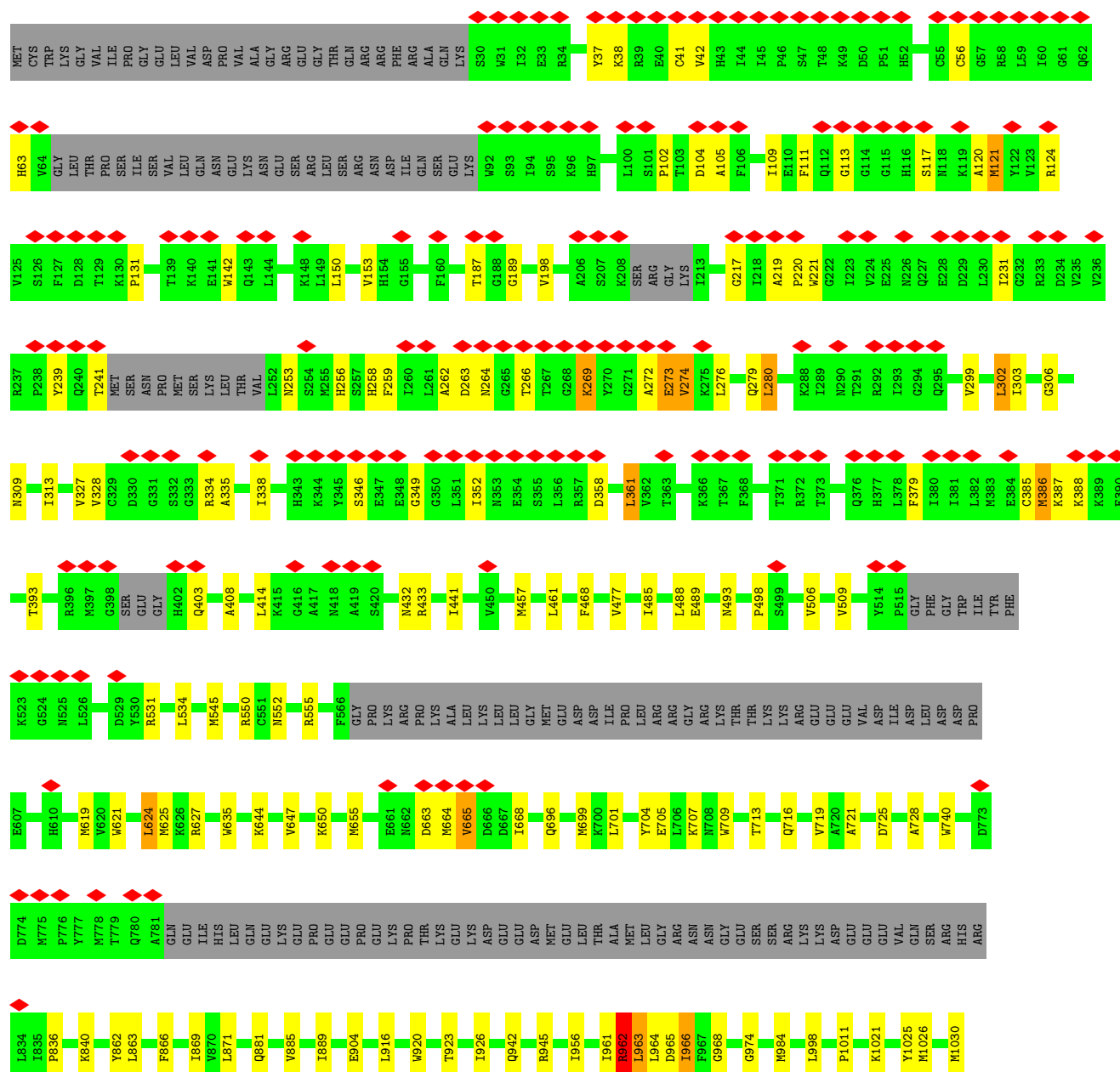


- Molecule 1: TRPM3

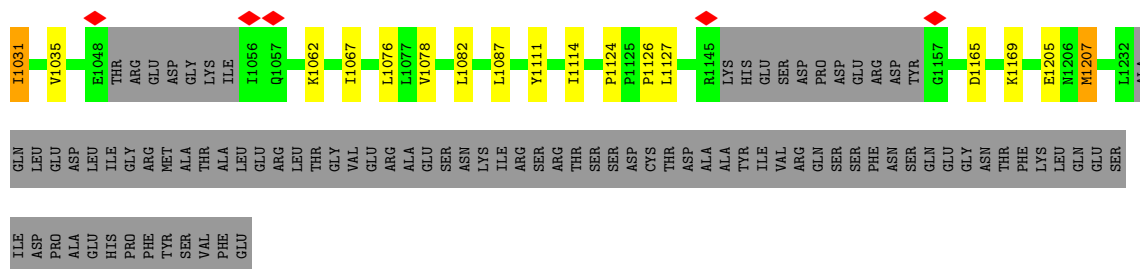




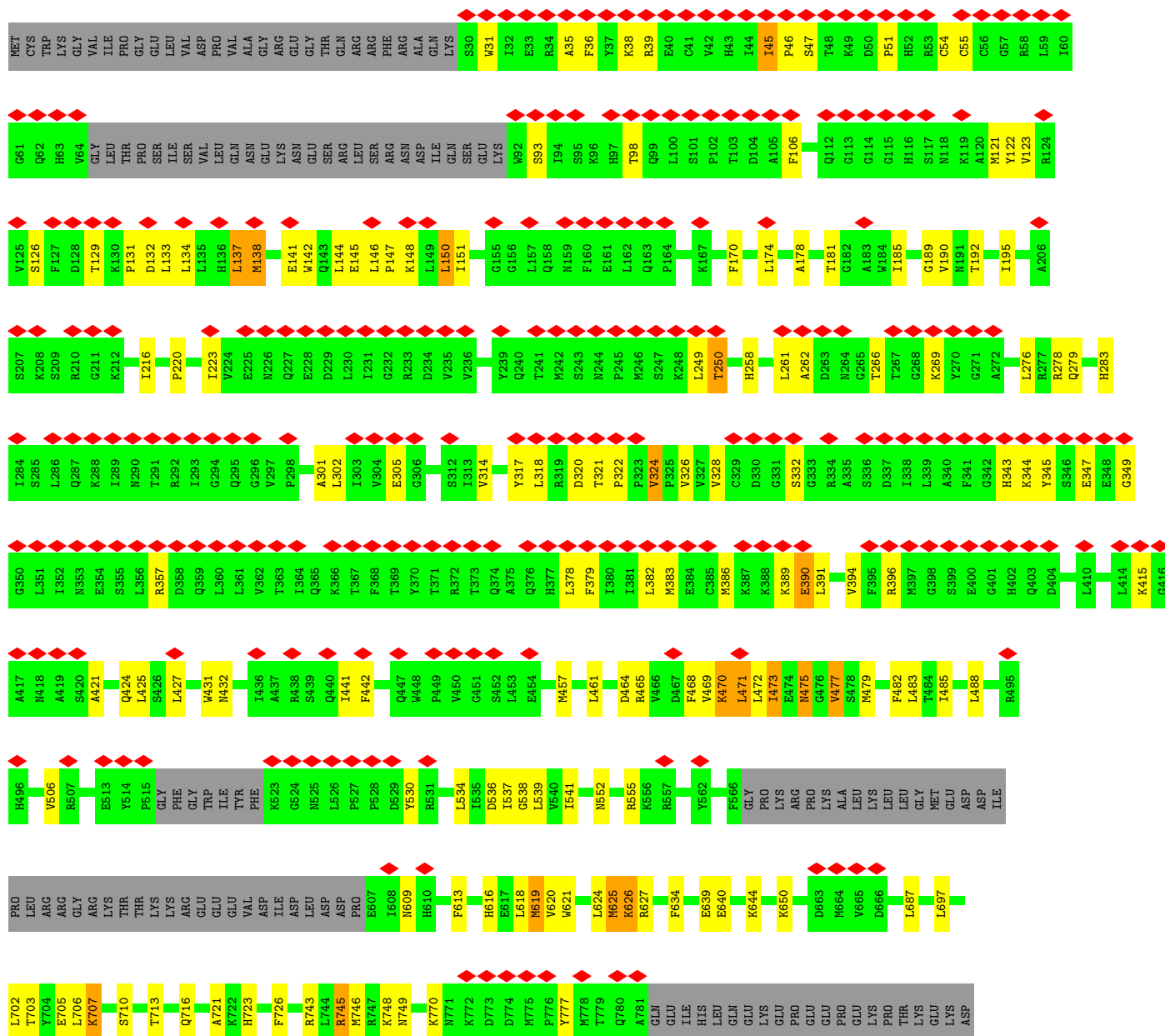
• Molecule 1: TRPM3

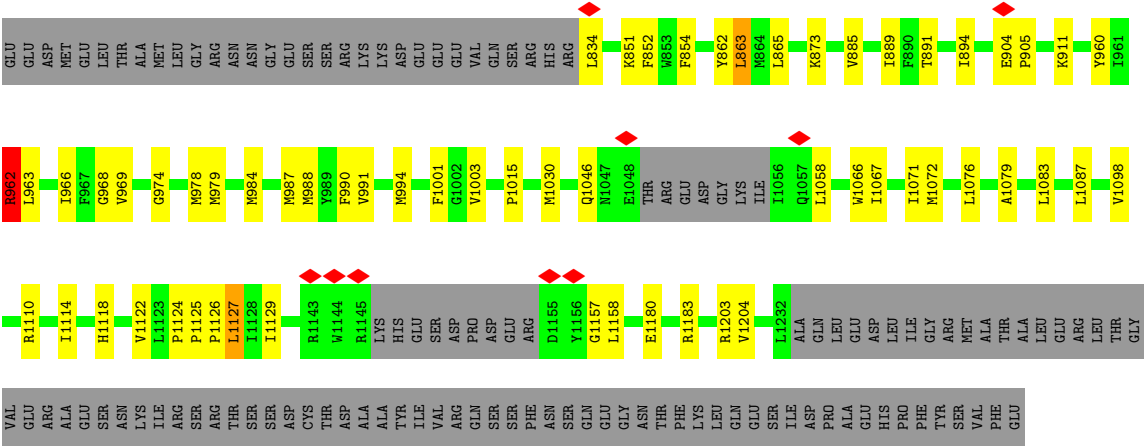






• Molecule 1: TRPM3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122730	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.013	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0039	Depositor
Map size ( $\text{\AA}$ )	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.826, 0.826, 0.826	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: Y01, A1AIA

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	0.46	1/7987 (0.0%)	0.88	6/10883 (0.1%)
1	B	0.45	1/7951 (0.0%)	0.85	4/10826 (0.0%)
1	C	0.48	0/8205	0.87	9/11167 (0.1%)
1	D	0.44	0/7965	0.86	9/10847 (0.1%)
All	All	0.46	2/32108 (0.0%)	0.87	28/43723 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	904	GLU	C-N	5.46	1.40	1.33
1	A	101	SER	C-N	5.12	1.39	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	834	LEU	CA-C-N	6.83	124.54	120.24
1	D	834	LEU	C-N-CA	6.83	124.54	120.24
1	A	1067	ILE	CA-C-N	6.54	124.36	120.24
1	A	1067	ILE	C-N-CA	6.54	124.36	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1067	ILE	CA-C-N	6.44	124.30	120.24
1	B	1067	ILE	C-N-CA	6.44	124.30	120.24
1	C	415	LYS	CG-CD-CE	6.30	125.80	111.30
1	A	1081	ILE	N-CA-C	-6.18	107.23	113.47
1	D	1067	ILE	CA-C-N	6.04	124.05	120.24
1	D	1067	ILE	C-N-CA	6.04	124.05	120.24
1	C	962	ARG	N-CA-C	-5.87	105.38	112.54
1	D	969	VAL	N-CA-C	-5.82	108.18	113.71
1	D	1179	GLU	N-CA-CB	5.75	118.67	110.16
1	C	145	GLU	CA-C-N	5.71	128.99	120.83
1	C	145	GLU	C-N-CA	5.71	128.99	120.83
1	B	408	ALA	N-CA-C	-5.70	106.12	114.39
1	D	287	GLN	N-CA-CB	5.68	119.02	109.94
1	A	102	PRO	N-CA-C	5.67	120.50	111.26
1	D	746	MET	CA-C-N	5.43	131.91	121.54
1	D	746	MET	C-N-CA	5.43	131.91	121.54
1	C	390	GLU	N-CA-C	-5.33	106.91	113.41
1	C	834	LEU	CA-C-N	5.20	123.51	120.24
1	C	834	LEU	C-N-CA	5.20	123.51	120.24
1	C	1067	ILE	CA-C-N	5.16	123.49	120.24
1	C	1067	ILE	C-N-CA	5.16	123.49	120.24
1	A	1122	VAL	CA-C-N	5.16	129.28	121.03
1	A	1122	VAL	C-N-CA	5.16	129.28	121.03
1	B	489	GLU	CA-CB-CG	5.08	124.27	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	962	ARG	Sidechain
1	C	396	ARG	Sidechain
1	C	962	ARG	Sidechain
1	D	1217	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7807	0	7248	96	0
1	B	7773	0	7249	109	0
1	C	8019	0	7670	151	0
1	D	7787	0	7251	102	0
2	A	210	0	294	4	0
2	B	245	0	343	9	0
2	C	175	0	245	4	0
2	D	210	0	294	6	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
All	All	32290	0	30594	456	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 (456) 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:107:GLY:CA	1:A:234:ASP:HA	1.77	1.13
1:A:107:GLY:HA2	1:A:234:ASP:HA	1.15	1.10
1:B:273:GLU:HA	1:B:276:LEU:HB3	1.55	0.88
1:A:107:GLY:HA2	1:A:234:ASP:CA	2.04	0.87
1:A:43:HIS:HE1	1:A:54:CYS:HB2	1.43	0.82
1:A:43:HIS:CE1	1:A:54:CYS:HB2	2.16	0.80
1:C:457:MET:HE1	1:C:472:LEU:HB3	1.64	0.79
1:D:327:VAL:HG21	1:D:408:ALA:HB1	1.69	0.74
1:B:550:ARG:HB3	1:B:555:ARG:HH22	1.54	0.72
1:C:189:GLY:H	1:C:195:ILE:HG12	1.55	0.71
1:A:624:LEU:HA	1:A:655:MET:HE1	1.76	0.68
1:C:469:VAL:HG22	1:C:473:ILE:HD12	1.75	0.68
1:B:624:LEU:HA	1:B:655:MET:HE1	1.77	0.67
1:D:406:ASP:HB3	1:D:433:ARG:HH12	1.59	0.67
1:A:153:VAL:HG22	1:A:302:LEU:HB2	1.77	0.67
1:B:111:PHE:HB3	1:B:241:THR:HG22	1.76	0.66
1:C:131:PRO:HG3	1:C:279:GLN:HB3	1.76	0.66
1:A:438:ARG:HB2	1:A:471:LEU:HD21	1.76	0.66
1:B:1030:MET:HE2	1:B:1076:LEU:HD21	1.78	0.65
1:C:479:MET:HA	1:C:482:PHE:HB3	1.78	0.65
1:C:390:GLU:HG2	1:C:391:LEU:HG	1.77	0.65
1:B:866:PHE:HD2	1:B:956:ILE:HD13	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:LEU:HB2	1:C:987:MET:HE1	1.79	0.65
1:D:149:LEU:HD13	1:D:413:LEU:HD21	1.78	0.64
1:B:105:ALA:HB2	1:B:231:ILE:HD12	1.79	0.64
1:C:301:ALA:HB3	1:C:326:VAL:HG22	1.79	0.64
1:B:352:ILE:HB	1:B:379:PHE:HE1	1.63	0.64
1:D:1203:ARG:HD2	1:C:1204:VAL:HG12	1.79	0.63
1:C:278:ARG:HH21	1:C:324:VAL:HG21	1.64	0.63
1:C:777:TYR:HB3	1:C:1158:LEU:HB3	1.80	0.63
1:B:650:LYS:HD3	1:B:721:ALA:HA	1.81	0.62
1:B:109:ILE:HG23	1:B:239:TYR:HB3	1.82	0.62
1:C:457:MET:HE3	1:C:473:ILE:HA	1.82	0.62
1:A:305:GLU:HG3	1:A:334:ARG:HD3	1.83	0.61
1:A:871:LEU:HD11	1:D:1023:ILE:HD11	1.82	0.61
1:C:713:THR:HB	1:C:716:GLN:HG3	1.83	0.60
1:D:314:VAL:O	1:D:318:LEU:HB2	2.02	0.60
1:C:39:ARG:HD2	1:C:126:SER:HB2	1.82	0.60
1:D:125:VAL:HG21	1:D:260:ILE:HG23	1.84	0.60
1:D:507:ARG:HB3	1:D:526:LEU:HB3	1.84	0.60
1:C:536:ASP:HA	1:C:539:LEU:HD12	1.83	0.60
1:B:272:ALA:C	1:B:274:VAL:H	2.10	0.59
1:B:37:TYR:HA	1:B:102:PRO:HA	1.83	0.59
1:C:151:ILE:HG21	1:C:174:LEU:HD11	1.85	0.59
1:C:483:LEU:HD11	1:C:488:LEU:HB2	1.85	0.59
1:C:865:LEU:HD11	2:C:1405:Y01:HAP2	1.84	0.59
1:C:266:THR:HB	1:C:269:LYS:HE2	1.84	0.59
1:D:195:ILE:HA	1:D:198:VAL:HG12	1.85	0.59
1:C:891:THR:HA	1:C:894:ILE:HD12	1.84	0.59
1:A:779:THR:HA	1:A:1157:GLY:HA2	1.84	0.59
1:D:713:THR:HB	1:D:716:GLN:HG3	1.83	0.59
1:C:968:GLY:HA2	1:C:974:GLY:HA2	1.85	0.58
1:D:424:GLN:HB3	1:D:441:ILE:HG12	1.84	0.58
1:C:862:TYR:HE1	1:C:885:VAL:HA	1.66	0.58
1:C:1046:GLN:HB2	1:C:1058:LEU:HD12	1.84	0.58
1:B:713:THR:HB	1:B:716:GLN:HG3	1.86	0.58
1:D:310:VAL:HA	1:D:313:ILE:HB	1.86	0.58
1:C:979:MET:HG2	1:C:1098:VAL:HG12	1.86	0.58
1:B:358:ASP:HA	1:B:361:LEU:HB2	1.86	0.58
1:A:1005:ARG:HG3	1:A:1009:LEU:HD12	1.86	0.57
1:B:266:THR:HB	1:B:269:LYS:HG3	1.85	0.57
1:A:189:GLY:H	1:A:195:ILE:HG12	1.69	0.57
1:D:411:THR:HG23	1:D:440:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1407:Y01:HAA2	1:C:991:VAL:HG13	1.86	0.57
1:C:442:PHE:CZ	1:C:472:LEU:HG	2.39	0.57
1:C:650:LYS:HD3	1:C:721:ALA:HA	1.87	0.57
1:C:1124:PRO:HB2	1:C:1126:PRO:HD2	1.87	0.57
1:D:190:VAL:HA	1:D:252:LEU:HA	1.86	0.57
1:D:304:VAL:HG12	1:D:329:CYS:HB2	1.87	0.57
1:C:46:PRO:HD2	1:C:54:CYS:HB2	1.87	0.57
1:C:121:MET:HE3	1:C:142:TRP:HA	1.87	0.57
1:C:344:LYS:HG3	1:C:345:TYR:HD2	1.70	0.57
1:A:346:SER:HA	1:A:352:ILE:HG23	1.87	0.57
1:A:429:LEU:HD21	1:A:460:ALA:HA	1.86	0.57
1:B:461:LEU:HB3	1:B:621:TRP:HH2	1.69	0.57
1:C:47:SER:HA	1:C:51:PRO:HA	1.87	0.56
1:C:618:LEU:HB3	1:C:634:PHE:CD2	2.40	0.56
1:A:107:GLY:CA	1:A:234:ASP:CA	2.69	0.56
1:A:485:ILE:HG23	1:A:534:LEU:HD12	1.86	0.56
1:D:465:ARG:HB3	1:D:468:PHE:HD2	1.70	0.56
1:B:1030:MET:HE3	1:B:1035:VAL:HA	1.85	0.56
1:C:318:LEU:HD22	1:C:391:LEU:HD12	1.87	0.56
1:D:56:CYS:HB2	1:D:266:THR:HA	1.88	0.56
1:B:346:SER:HB2	1:B:349:GLY:HA2	1.88	0.56
1:D:222:GLY:HA3	1:D:267:THR:HA	1.88	0.56
1:B:963:LEU:HA	1:B:966:ILE:HG13	1.87	0.56
1:A:619:MET:HE3	1:A:644:LYS:HB3	1.88	0.56
1:D:942:GLN:HG2	1:D:945:ARG:HE	1.71	0.56
1:D:184:TRP:CD1	1:D:214:CYS:HG	2.23	0.56
1:C:170:PHE:HE1	1:C:302:LEU:HD21	1.71	0.56
1:C:640:GLU:O	1:C:644:LYS:HG3	2.06	0.55
1:C:138:MET:HE1	1:C:216:ILE:HG12	1.88	0.55
1:B:619:MET:HE3	1:B:644:LYS:HB3	1.86	0.55
2:A:1402:Y01:HAB2	1:B:863:LEU:HD23	1.88	0.55
1:A:668:ILE:HA	1:A:671:GLU:HG2	1.88	0.54
1:A:1124:PRO:HD2	1:A:1127:LEU:HB2	1.88	0.54
1:D:850:VAL:O	1:D:854:PHE:HB2	2.08	0.54
1:A:506:VAL:HA	1:A:509:VAL:HG12	1.89	0.54
1:A:619:MET:HE1	1:A:635:TRP:HA	1.88	0.54
1:C:121:MET:HB2	1:C:258:HIS:HD2	1.72	0.54
1:B:38:LYS:HG2	1:B:124:ARG:HH21	1.72	0.54
1:A:941:ASP:HA	1:A:945:ARG:NH1	2.22	0.54
1:C:46:PRO:HD2	1:C:55:CYS:H	1.71	0.54
1:D:1021:LYS:O	1:D:1025:TYR:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:HG22	1:C:431:TRP:HB3	1.89	0.54
1:B:1078:VAL:HG21	2:B:1408:Y01:HAP1	1.88	0.54
1:C:45:ILE:HA	1:C:54:CYS:HB3	1.88	0.54
1:B:306:GLY:H	1:B:334:ARG:HH21	1.54	0.54
1:C:465:ARG:HB3	1:C:468:PHE:HD1	1.73	0.53
1:D:349:GLY:HA3	1:D:387:LYS:HA	1.89	0.53
1:C:35:ALA:HB1	1:C:133:LEU:HD11	1.91	0.53
1:C:457:MET:HG3	1:C:477:VAL:HB	1.91	0.53
1:D:889:ILE:HG23	1:D:928:ILE:HG12	1.91	0.53
1:C:321:THR:HB	1:C:322:PRO:HD3	1.90	0.53
1:C:618:LEU:HB3	1:C:634:PHE:CE2	2.43	0.53
1:D:1203:ARG:O	1:D:1207:MET:HG2	2.09	0.53
1:C:468:PHE:O	1:C:472:LEU:N	2.37	0.53
1:A:266:THR:HB	1:A:269:LYS:HD2	1.91	0.53
1:A:1021:LYS:O	1:A:1025:TYR:HB2	2.09	0.53
1:D:545:MET:HE1	1:D:647:VAL:HG13	1.91	0.53
1:C:485:ILE:HG13	1:C:609:ASN:HA	1.90	0.53
1:C:613:PHE:HB3	1:C:616:HIS:HD1	1.73	0.53
1:C:613:PHE:HB3	1:C:616:HIS:ND1	2.23	0.53
1:C:748:LYS:O	1:C:749:ASN:C	2.51	0.53
1:A:1111:TYR:O	1:A:1115:MET:HG2	2.09	0.53
1:B:187:THR:H	1:B:217:GLY:HA2	1.73	0.53
1:C:621:TRP:CE2	1:C:625:MET:HE1	2.44	0.53
1:C:1015:PRO:HB3	2:C:1403:Y01:HAV1	1.89	0.53
1:C:328:VAL:HB	1:C:394:VAL:HG22	1.90	0.52
1:A:151:ILE:HB	1:A:185:ILE:HA	1.92	0.52
1:C:904:GLU:CB	1:C:911:LYS:HA	2.39	0.52
1:B:665:VAL:O	1:B:668:ILE:HG22	2.09	0.52
1:A:31:TRP:CZ3	1:A:137:LEU:HB2	2.45	0.52
1:A:866:PHE:HA	1:A:869:ILE:HG12	1.91	0.52
1:C:457:MET:HE3	1:C:473:ILE:HG13	1.90	0.52
1:A:325:PRO:HA	1:A:391:LEU:HB3	1.91	0.52
1:B:41:CYS:HB2	1:B:63:HIS:HA	1.90	0.52
1:B:457:MET:HG3	1:B:477:VAL:HG11	1.91	0.52
1:C:538:GLY:HA2	1:C:541:ILE:HD12	1.91	0.52
1:B:221:TRP:HB3	1:B:263:ASP:HA	1.91	0.52
1:B:506:VAL:HA	1:B:509:VAL:HG22	1.91	0.52
1:B:1124:PRO:HD2	1:B:1127:LEU:HB2	1.92	0.52
1:A:949:ARG:NH1	1:D:1011:PRO:HA	2.25	0.52
1:D:318:LEU:HD22	1:D:388:LYS:HD2	1.92	0.52
1:D:352:ILE:H	1:D:379:PHE:HZ	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:LEU:HA	1:C:537:ILE:HD12	1.91	0.52
1:A:294:GLY:HA2	1:A:419:ALA:HB2	1.92	0.51
1:C:555:ARG:HH22	1:C:710:SER:HA	1.75	0.51
1:A:942:GLN:HG2	1:A:945:ARG:HB3	1.92	0.51
1:B:56:CYS:HB3	1:B:266:THR:HA	1.91	0.51
1:C:31:TRP:CZ3	1:C:137:LEU:HB2	2.46	0.51
1:A:112:GLN:HB3	1:A:238:PRO:O	2.11	0.51
1:B:701:LEU:HD12	1:B:704:TYR:HE1	1.75	0.51
1:B:104:ASP:HB2	1:B:124:ARG:HH22	1.76	0.51
1:C:305:GLU:HG3	1:C:332:SER:HB2	1.92	0.51
1:C:865:LEU:HD21	2:C:1405:Y01:HAQ2	1.93	0.51
1:D:350:GLY:CA	1:D:386:MET:HB3	2.41	0.51
1:D:500:ASN:ND2	1:D:502:LEU:HB2	2.26	0.51
1:D:1115:MET:HE1	1:D:1158:LEU:HG	1.92	0.51
1:B:1021:LYS:O	1:B:1025:TYR:HB2	2.11	0.51
1:D:920:TRP:HB3	1:D:962:ARG:HH12	1.76	0.50
1:B:113:GLY:H	1:C:475:ASN:HB3	1.75	0.50
1:B:385:CYS:SG	1:B:386:MET:N	2.84	0.50
1:C:506:VAL:HG11	1:C:530:TYR:HE2	1.75	0.50
1:D:500:ASN:ND2	1:D:625:MET:HA	2.26	0.50
1:D:151:ILE:HB	1:D:185:ILE:HA	1.94	0.50
1:D:390:GLU:HG2	1:D:391:LEU:HD22	1.92	0.50
1:C:36:PHE:HZ	1:C:134:LEU:HA	1.75	0.50
1:C:851:LYS:HE2	1:C:1122:VAL:HA	1.94	0.50
1:B:942:GLN:OE1	1:B:945:ARG:HB3	2.12	0.50
1:C:421:ALA:HA	1:C:424:GLN:HB2	1.94	0.50
1:B:414:LEU:HD13	1:B:441:ILE:HD11	1.94	0.50
1:B:619:MET:HE1	1:B:635:TRP:HA	1.94	0.50
1:B:836:PRO:O	1:B:840:LYS:HB2	2.12	0.50
1:B:962:ARG:O	1:B:963:LEU:C	2.55	0.50
1:B:120:ALA:HB1	1:B:259:PHE:HE2	1.77	0.50
1:C:854:PHE:CE2	1:C:1124:PRO:HD3	2.47	0.50
1:D:315:LEU:HD12	1:D:388:LYS:NZ	2.27	0.49
1:B:327:VAL:HA	1:B:393:THR:HB	1.94	0.49
1:D:1006:GLN:O	1:D:1010:PHE:HB2	2.11	0.49
1:B:120:ALA:HB1	1:B:259:PHE:CE2	2.47	0.49
1:D:220:PRO:HG2	1:D:270:TYR:HA	1.94	0.49
1:D:1110:ARG:O	1:D:1114:ILE:HG12	2.13	0.49
1:B:552:ASN:HA	1:B:555:ARG:HG2	1.94	0.49
1:A:301:ALA:HB3	1:A:326:VAL:HG23	1.93	0.49
1:B:923:THR:HA	1:B:926:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLY:HA3	1:B:219:ALA:HB2	1.94	0.49
1:A:239:TYR:OH	1:A:251:VAL:HG23	2.13	0.49
1:C:36:PHE:HE1	1:C:133:LEU:HG	1.77	0.49
1:B:862:TYR:HE1	1:B:885:VAL:HG13	1.77	0.49
1:B:150:LEU:HB2	1:B:299:VAL:HA	1.94	0.49
1:B:696:GLN:HA	1:B:699:MET:HG2	1.95	0.49
1:B:866:PHE:HD1	1:B:885:VAL:HG11	1.78	0.49
1:A:202:LEU:HA	1:A:205:HIS:CD2	2.48	0.48
1:D:886:ILE:HG12	1:D:935:MET:SD	2.52	0.48
1:A:492:TYR:HE2	1:A:624:LEU:HD12	1.77	0.48
1:A:109:ILE:HG23	1:A:239:TYR:HB3	1.95	0.48
1:A:309:ASN:O	1:A:313:ILE:HG23	2.13	0.48
1:A:915:TRP:HH2	1:A:925:LEU:HB2	1.79	0.48
1:C:122:TYR:HB2	1:C:261:LEU:HD11	1.94	0.48
1:C:220:PRO:HB2	1:C:223:ILE:HG22	1.95	0.48
1:C:192:THR:HG23	1:C:250:THR:HG21	1.95	0.48
1:D:642:MET:HE3	1:D:686:LEU:HD23	1.95	0.48
1:B:998:LEU:HD12	1:B:1031:ILE:HD11	1.96	0.48
1:A:886:ILE:HG12	1:A:935:MET:SD	2.54	0.48
1:C:625:MET:HE3	1:C:627:ARG:HH11	1.79	0.48
1:C:963:LEU:HD23	1:C:963:LEU:HA	1.78	0.48
1:D:315:LEU:HD12	1:D:388:LYS:HZ1	1.78	0.48
1:C:314:VAL:O	1:C:318:LEU:HG	2.13	0.48
1:A:1078:VAL:HG23	1:A:1082:LEU:HD23	1.95	0.48
1:C:137:LEU:HA	1:C:141:GLU:OE1	2.14	0.48
1:D:905:PRO:HG2	1:D:914:VAL:HG21	1.95	0.48
1:D:1085:ASN:HA	1:D:1088:ILE:HG12	1.96	0.48
1:B:386:MET:O	1:B:387:LYS:C	2.57	0.48
1:B:866:PHE:HA	1:B:869:ILE:HG12	1.96	0.48
1:C:705:GLU:HG2	1:C:707:LYS:HD3	1.95	0.48
1:A:1164:ASP:HA	1:A:1167:LEU:HB3	1.96	0.47
1:C:190:VAL:HB	1:C:250:THR:HB	1.96	0.47
1:A:736:LEU:HD21	1:A:1111:TYR:HD1	1.79	0.47
1:A:769:PHE:HZ	1:A:844:PHE:HB2	1.78	0.47
1:A:1124:PRO:HB2	1:A:1126:PRO:HD2	1.95	0.47
1:A:949:ARG:NH1	1:D:1007:ALA:O	2.47	0.47
2:D:1406:Y01:HAP1	2:D:1406:Y01:HAO2	1.42	0.47
1:C:471:LEU:HD12	1:C:472:LEU:HD12	1.96	0.47
1:A:220:PRO:HG3	1:A:270:TYR:HA	1.96	0.47
1:B:273:GLU:O	1:B:274:VAL:C	2.58	0.47
1:B:488:LEU:HD23	1:B:534:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:ARG:O	1:B:964:LEU:N	2.47	0.47
1:C:990:PHE:HB2	1:C:1087:LEU:HD13	1.97	0.47
1:B:1205:GLU:HA	1:C:1203:ARG:HH12	1.80	0.47
1:C:707:LYS:HE2	1:C:707:LYS:HB2	1.52	0.47
1:A:998:LEU:HG	1:A:1027:PRO:HB2	1.96	0.47
1:B:881:GLN:HE21	2:B:1405:Y01:HAI	1.78	0.47
1:C:616:HIS:HE1	1:C:639:GLU:HB3	1.80	0.47
1:A:149:LEU:HD13	1:A:413:LEU:HD12	1.97	0.47
1:A:151:ILE:HG21	1:A:174:LEU:HD11	1.96	0.47
1:D:202:LEU:HD23	1:D:255:MET:HG3	1.96	0.47
1:D:1029:TRP:CH2	1:C:1072:MET:HG2	2.50	0.47
1:B:493:ASN:HD22	1:B:531:ARG:HH11	1.63	0.47
1:B:920:TRP:HH2	1:B:961:ILE:HG22	1.79	0.47
1:D:987:MET:HB2	1:D:987:MET:HE3	1.70	0.47
1:B:740:TRP:CE3	1:B:1114:ILE:HG13	2.50	0.47
1:C:148:LYS:HB3	1:C:431:TRP:CD1	2.50	0.47
1:C:469:VAL:HA	1:C:473:ILE:HB	1.97	0.47
1:A:889:ILE:HG23	1:A:928:ILE:HG12	1.97	0.46
1:D:335:ALA:HA	1:D:338:ILE:HG12	1.97	0.46
1:D:641:ALA:HA	1:D:644:LYS:HD3	1.96	0.46
1:B:725:ASP:HA	1:B:728:ALA:HB3	1.96	0.46
1:B:1026:MET:O	1:B:1030:MET:HG3	2.14	0.46
1:C:457:MET:HE3	1:C:473:ILE:CA	2.44	0.46
1:A:329:CYS:HA	1:A:395:PHE:HB3	1.97	0.46
1:B:272:ALA:C	1:B:274:VAL:N	2.73	0.46
1:C:1180:GLU:HA	1:C:1183:ARG:HG2	1.96	0.46
1:D:325:PRO:HA	1:D:391:LEU:HB3	1.97	0.46
1:C:534:LEU:HD23	1:C:537:ILE:HD12	1.97	0.46
1:C:626:LYS:HE3	1:C:626:LYS:HB3	1.34	0.46
1:C:984:MET:O	1:C:988:MET:HG2	2.15	0.46
1:C:1066:TRP:HB3	2:C:1401:Y01:HAM2	1.98	0.46
1:B:121:MET:HG3	1:B:142:TRP:CE2	2.51	0.46
1:B:335:ALA:HA	1:B:338:ILE:HG12	1.96	0.46
1:A:237:ARG:C	1:A:239:TYR:H	2.24	0.46
1:D:863:LEU:HD12	1:D:863:LEU:HA	1.72	0.46
1:C:745:ARG:CZ	1:C:770:LYS:HA	2.46	0.46
1:D:109:ILE:HD13	1:D:237:ARG:HB2	1.97	0.46
1:C:343:HIS:HA	1:C:386:MET:HE1	1.98	0.46
1:C:468:PHE:HB3	1:C:472:LEU:HD22	1.98	0.46
1:C:862:TYR:CE1	1:C:885:VAL:HA	2.50	0.46
1:D:703:THR:HG23	1:D:735:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD22	1:A:413:LEU:HD12	1.99	0.46
1:D:232:GLY:HA3	1:D:237:ARG:HE	1.81	0.46
1:C:178:ALA:HB2	1:C:185:ILE:HD11	1.98	0.46
1:C:743:ARG:HH11	1:C:770:LYS:HD2	1.80	0.46
1:B:272:ALA:O	1:B:274:VAL:N	2.49	0.45
1:C:552:ASN:HA	1:C:555:ARG:HG3	1.98	0.45
2:A:1405:Y01:HAO2	2:A:1405:Y01:HAP1	1.41	0.45
1:C:979:MET:HE2	1:C:979:MET:HB3	1.54	0.45
1:A:105:ALA:HA	1:A:232:GLY:H	1.81	0.45
1:B:276:LEU:HD12	1:B:279:GLN:HE21	1.82	0.45
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.84	0.45
1:D:46:PRO:HD2	1:D:55:CYS:N	2.31	0.45
1:A:1009:LEU:HD11	1:A:1068:VAL:HG11	1.99	0.45
1:B:968:GLY:HA2	1:B:974:GLY:HA2	1.99	0.45
2:B:1403:Y01:HAP1	2:B:1403:Y01:HAO2	1.64	0.45
1:C:470:LYS:HE3	1:C:470:LYS:HB2	1.48	0.45
1:B:121:MET:HB2	1:B:258:HIS:HD2	1.82	0.45
1:C:987:MET:HB2	1:C:987:MET:HE3	1.70	0.45
1:B:962:ARG:C	1:B:964:LEU:N	2.74	0.45
1:B:309:ASN:O	1:B:313:ILE:HG12	2.17	0.44
2:B:1405:Y01:HAP1	2:B:1405:Y01:HAO2	1.42	0.44
1:C:960:TYR:O	1:C:963:LEU:HB2	2.15	0.44
1:A:1078:VAL:HG21	2:B:1403:Y01:HAP1	1.98	0.44
1:D:124:ARG:HG2	1:D:221:TRP:CD2	2.53	0.44
1:D:616:HIS:NE2	1:D:640:GLU:HB2	2.33	0.44
1:B:705:GLU:HG2	1:B:707:LYS:HD3	1.98	0.44
1:B:1124:PRO:HB2	1:B:1126:PRO:HD2	1.99	0.44
1:D:109:ILE:HG12	1:D:122:TYR:CD1	2.52	0.44
1:B:866:PHE:HE2	1:B:956:ILE:HB	1.82	0.44
1:C:1110:ARG:O	1:C:1114:ILE:HG12	2.17	0.44
1:A:1207:MET:HE3	1:B:1207:MET:HE1	2.00	0.44
1:D:912:VAL:O	1:D:916:LEU:HG	2.17	0.44
1:B:963:LEU:HA	1:B:963:LEU:HD12	1.81	0.44
1:C:994:MET:HE1	1:C:1079:ALA:HA	2.00	0.44
1:B:153:VAL:HG22	1:B:302:LEU:HD21	1.99	0.44
1:A:43:HIS:HB3	1:A:96:LYS:O	2.18	0.44
1:D:32:ILE:HD11	1:D:141:GLU:HG2	2.00	0.43
1:B:719:VAL:HG21	1:B:1111:TYR:CD2	2.52	0.43
1:A:898:ARG:HE	1:A:1135:MET:HE2	1.83	0.43
1:A:995:LEU:HD23	1:A:995:LEU:HA	1.88	0.43
1:D:296:GLY:O	1:D:297:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:PRO:HB3	1:D:452:SER:HB2	1.99	0.43
1:D:854:PHE:HE2	1:D:1124:PRO:HD3	1.83	0.43
1:A:454:GLU:HG2	1:A:487:ARG:HH12	1.83	0.43
1:C:383:MET:HA	1:C:386:MET:HB2	1.99	0.43
1:A:107:GLY:HA3	1:A:234:ASP:HA	1.88	0.43
1:A:1059:PRO:HA	1:A:1060:PRO:HD3	1.89	0.43
1:D:93:SER:HA	1:D:97:HIS:HA	2.00	0.43
1:B:545:MET:SD	1:B:647:VAL:HG13	2.58	0.43
1:B:881:GLN:NE2	2:B:1405:Y01:HAI	2.32	0.43
2:B:1408:Y01:HAP1	2:B:1408:Y01:HAO2	1.69	0.43
1:C:220:PRO:HA	1:C:262:ALA:HB3	1.99	0.43
1:C:1030:MET:HB3	1:C:1076:LEU:HD21	2.00	0.43
1:D:41:CYS:HA	1:D:98:THR:HA	2.00	0.43
1:D:473:ILE:O	1:D:474:GLU:C	2.62	0.43
1:B:619:MET:HB2	1:B:619:MET:HE2	1.74	0.43
1:C:618:LEU:HD13	1:C:634:PHE:CZ	2.53	0.43
1:C:687:LEU:HD13	1:C:702:LEU:HD21	2.00	0.43
1:C:697:LEU:HD23	1:C:697:LEU:HA	1.90	0.43
1:A:106:PHE:HB3	1:A:123:VAL:HG23	2.00	0.43
1:D:221:TRP:HA	1:D:261:LEU:HG	2.01	0.43
1:D:705:GLU:HG2	1:D:707:LYS:HD2	2.01	0.43
1:D:881:GLN:NE2	2:D:1406:Y01:HAI	2.33	0.43
1:C:425:LEU:HB3	1:C:441:ILE:HG21	2.00	0.43
1:C:978:MET:HE3	1:C:978:MET:HB3	1.84	0.43
2:D:1404:Y01:HAP1	2:D:1404:Y01:HAO2	1.71	0.43
1:B:220:PRO:HA	1:B:272:ALA:HB3	2.01	0.43
1:C:93:SER:HA	1:C:98:THR:H	1.83	0.43
1:C:468:PHE:O	1:C:472:LEU:HB2	2.18	0.43
1:C:625:MET:HE2	1:C:625:MET:HB2	1.76	0.43
1:A:46:PRO:O	1:A:54:CYS:HA	2.18	0.43
2:A:1403:Y01:HAO2	2:A:1403:Y01:HAP1	1.66	0.43
1:D:854:PHE:CE2	1:D:1124:PRO:HD3	2.53	0.43
1:C:38:LYS:HA	1:C:126:SER:HB3	2.00	0.43
1:C:432:ASN:HA	1:C:465:ARG:NH1	2.34	0.43
1:A:941:ASP:HA	1:A:945:ARG:HH12	1.82	0.43
1:A:951:ILE:O	1:A:952:TYR:C	2.62	0.43
1:D:232:GLY:HA3	1:D:237:ARG:HH21	1.84	0.43
1:B:111:PHE:HB2	1:B:117:SER:HA	2.01	0.43
1:C:905:PRO:O	1:C:911:LYS:HG3	2.19	0.43
1:C:1118:HIS:CE1	1:C:1158:LEU:HD21	2.53	0.43
1:A:39:ARG:HB3	1:A:98:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:O	1:A:313:ILE:HG12	2.18	0.42
1:A:953:CYS:HB2	1:D:1008:ILE:HD11	2.01	0.42
1:D:279:GLN:O	1:D:282:LYS:HG2	2.19	0.42
1:D:630:MET:HB2	1:D:630:MET:HE2	1.71	0.42
2:D:1401:Y01:HAC3	2:D:1401:Y01:HAJ2	1.81	0.42
1:C:146:LEU:HD12	1:C:147:PRO:HD2	2.00	0.42
1:C:349:GLY:HA2	1:C:389:LYS:HD3	2.00	0.42
1:C:357:ARG:HG3	1:C:379:PHE:CZ	2.54	0.42
1:A:56:CYS:C	1:A:58:ARG:H	2.27	0.42
1:A:1084:VAL:O	1:A:1088:ILE:HD12	2.20	0.42
1:D:888:TYR:CD2	1:D:1126:PRO:HD3	2.54	0.42
1:B:1011:PRO:HD3	1:B:1062:LYS:HG2	2.01	0.42
1:C:138:MET:HG3	1:C:144:LEU:HD12	2.00	0.42
1:B:253:ASN:HB3	1:B:256:HIS:HD1	1.84	0.42
1:C:963:LEU:HD23	1:C:966:ILE:HG13	2.01	0.42
1:A:534:LEU:HA	1:A:537:ILE:HG12	2.00	0.42
1:D:473:ILE:C	1:D:475:ASN:N	2.77	0.42
1:C:461:LEU:HB3	1:C:621:TRP:CH2	2.54	0.42
1:C:703:THR:HA	1:C:713:THR:HG23	2.00	0.42
1:B:386:MET:HB2	1:B:386:MET:HE2	1.79	0.42
1:B:432:ASN:HA	1:B:468:PHE:HE2	1.83	0.42
1:A:199:GLY:HA3	1:A:253:ASN:HD21	1.85	0.42
1:A:853:TRP:HA	1:A:856:THR:HG22	2.01	0.42
1:B:433:ARG:HD2	1:B:433:ARG:HA	1.83	0.42
1:C:132:ASP:HA	1:C:283:HIS:CE1	2.55	0.42
1:D:625:MET:O	1:D:627:ARG:HG3	2.20	0.42
1:D:736:LEU:HD21	1:D:1111:TYR:HD1	1.84	0.42
1:B:461:LEU:HB3	1:B:621:TRP:CH2	2.53	0.42
1:A:233:ARG:O	1:A:234:ASP:C	2.62	0.42
1:A:238:PRO:O	1:A:239:TYR:C	2.63	0.42
1:A:626:LYS:HZ2	1:A:626:LYS:HG3	1.57	0.42
1:A:701:LEU:HD12	1:A:704:TYR:HE1	1.85	0.42
1:C:223:ILE:HD12	1:C:249:LEU:HG	2.02	0.42
1:B:303:ILE:HB	1:B:328:VAL:HG12	2.01	0.42
1:B:664:MET:O	1:B:665:VAL:C	2.63	0.42
1:D:745:ARG:O	1:D:747:ARG:HD2	2.20	0.42
1:C:427:LEU:HD23	1:C:427:LEU:HA	1.95	0.42
1:C:716:GLN:NE2	1:C:1157:GLY:HA3	2.35	0.42
1:C:1127:LEU:C	1:C:1129:ILE:N	2.78	0.42
1:D:108:THR:HA	1:D:121:MET:HA	2.02	0.41
1:D:1030:MET:HB3	1:D:1076:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:MET:HE3	1:B:984:MET:HB3	1.93	0.41
1:C:106:PHE:HB2	1:C:123:VAL:HG22	2.01	0.41
1:A:378:LEU:O	1:A:382:LEU:HB2	2.19	0.41
1:B:253:ASN:HB3	1:B:256:HIS:ND1	2.35	0.41
1:C:620:VAL:O	1:C:624:LEU:HB2	2.19	0.41
1:C:1001:PHE:HE1	1:C:1071:ILE:HG13	1.84	0.41
1:A:469:VAL:O	1:A:473:ILE:HG12	2.19	0.41
1:C:36:PHE:CE1	1:C:133:LEU:HG	2.56	0.41
1:A:43:HIS:N	1:A:63:HIS:HE1	2.18	0.41
1:D:104:ASP:HA	1:D:233:ARG:HB3	2.02	0.41
1:C:1158:LEU:HD23	1:C:1158:LEU:HA	1.89	0.41
1:D:45:ILE:HG23	1:D:63:HIS:CE1	2.56	0.41
1:D:305:GLU:H	1:D:336:SER:HB3	1.86	0.41
1:D:871:LEU:HD21	1:C:1003:VAL:HG13	2.03	0.41
1:D:979:MET:HE1	1:D:1095:PHE:CD1	2.56	0.41
1:A:613:PHE:HB3	1:A:616:HIS:HD1	1.86	0.41
1:D:175:ILE:O	1:D:179:MET:HG2	2.21	0.41
1:D:868:TYR:CD2	2:D:1405:Y01:HAI	2.55	0.41
1:B:863:LEU:HD12	1:B:863:LEU:HA	1.95	0.41
1:D:170:PHE:HE1	1:D:302:LEU:HD11	1.86	0.41
1:A:322:PRO:HA	1:A:323:PRO:HD3	1.97	0.41
1:A:725:ASP:HA	1:A:728:ALA:HB3	2.02	0.41
1:B:647:VAL:HG11	1:B:709:TRP:CZ3	2.55	0.41
1:B:862:TYR:CZ	1:B:889:ILE:HD11	2.55	0.41
1:B:1087:LEU:HD12	1:B:1087:LEU:HA	1.87	0.41
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.86	0.41
1:C:723:HIS:CD2	1:C:726:PHE:HB2	2.56	0.41
1:D:330:ASP:HB3	1:D:340:ALA:HB2	2.02	0.41
1:C:322:PRO:HG2	1:C:324:VAL:HG22	2.03	0.41
1:A:425:LEU:HA	1:A:441:ILE:HD13	2.03	0.41
1:A:975:PRO:O	1:A:979:MET:HB2	2.21	0.41
1:D:382:LEU:HA	1:D:385:CYS:HB2	2.03	0.41
1:D:744:LEU:HD21	1:D:844:PHE:HD1	1.86	0.41
1:B:485:ILE:HG23	1:B:534:LEU:HD13	2.03	0.41
2:B:1401:Y01:HAP1	2:B:1401:Y01:HAO2	1.78	0.41
1:C:129:THR:H	1:C:276:LEU:HD21	1.86	0.41
1:C:278:ARG:HA	1:C:278:ARG:HD2	1.66	0.41
1:C:863:LEU:HD12	1:C:863:LEU:HA	1.83	0.41
1:A:222:GLY:HA3	1:A:267:THR:HA	2.02	0.40
1:A:889:ILE:HD13	1:A:889:ILE:HA	1.86	0.40
1:A:1023:ILE:HD11	1:B:871:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:LEU:HA	1:D:655:MET:HE1	2.04	0.40
1:B:498:PRO:HD2	1:B:627:ARG:HH21	1.86	0.40
1:C:852:PHE:CE1	1:C:969:VAL:HG21	2.56	0.40
1:A:754:VAL:HG13	1:A:850:VAL:HG22	2.03	0.40
1:D:135:LEU:HD13	1:D:135:LEU:HA	1.94	0.40
1:B:262:ALA:HB3	1:B:272:ALA:HB1	2.02	0.40
1:B:1165:ASP:O	1:B:1169:LYS:HG2	2.22	0.40
1:A:256:HIS:HB2	1:A:259:PHE:CZ	2.57	0.40
1:D:619:MET:O	1:D:623:VAL:HG23	2.21	0.40
1:D:776:PRO:HB2	1:D:778:MET:HE3	2.02	0.40
2:D:1405:Y01:HAA1	2:D:1405:Y01:HAJ1	1.93	0.40
1:B:264:ASN:CG	1:B:272:ALA:HB2	2.45	0.40
1:C:1125:PRO:N	1:C:1126:PRO:HD2	2.36	0.40
1:D:280:LEU:O	1:D:284:ILE:HG12	2.22	0.40
1:D:1087:LEU:HD12	1:D:1087:LEU:HA	1.86	0.40
1:B:131:PRO:HB3	1:B:280:LEU:HG	2.03	0.40
1:C:278:ARG:HD3	1:C:317:TYR:CE1	2.57	0.40
1:C:619:MET:HB2	1:C:619:MET:HE3	1.67	0.40
1:C:1083:LEU:HD23	1:C:1083:LEU:HA	1.89	0.40
1:A:1092:ASN:ND2	1:D:1093[A]:ASN:ND2	2.70	0.40
2:A:1407:Y01:HAB1	2:A:1407:Y01:HAJ1	1.92	0.40
1:D:45:ILE:HG22	1:D:54:CYS:HB3	2.03	0.40
1:B:153:VAL:HG11	1:B:198:VAL:HG21	2.03	0.40
1:C:889:ILE:HA	1:C:889:ILE:HD13	1.80	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	1035/1306 (79%)	964 (93%)	71 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1024/1306 (78%)	948 (93%)	73 (7%)	3 (0%)	37	69
1	C	1048/1306 (80%)	966 (92%)	81 (8%)	1 (0%)	48	79
1	D	1027/1306 (79%)	954 (93%)	73 (7%)	0	100	100
All	All	4134/5224 (79%)	3832 (93%)	298 (7%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	GLU
1	B	963	LEU
1	C	347	GLU
1	B	665	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	743/1162 (64%)	727 (98%)	16 (2%)	47	70
1	B	742/1162 (64%)	723 (97%)	19 (3%)	41	66
1	C	792/1162 (68%)	767 (97%)	25 (3%)	34	62
1	D	743/1162 (64%)	734 (99%)	9 (1%)	67	81
All	All	3020/4648 (65%)	2951 (98%)	69 (2%)	46	69

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	CYS
1	A	137	LEU
1	A	235	VAL
1	A	236	VAL
1	A	362	VAL
1	A	386	MET
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	472	LEU
1	A	668	ILE
1	A	916	LEU
1	A	940	GLN
1	A	941	ASP
1	A	949	ARG
1	A	965	ASP
1	A	966	ILE
1	A	1166	GLU
1	D	413	LEU
1	D	429	LEU
1	D	472	LEU
1	D	475	ASN
1	D	619	MET
1	D	863	LEU
1	D	864	MET
1	D	1167	LEU
1	D	1217	ARG
1	B	42	VAL
1	B	121	MET
1	B	269	LYS
1	B	274	VAL
1	B	280	LEU
1	B	302	LEU
1	B	361	LEU
1	B	386	MET
1	B	388	LYS
1	B	403	GLN
1	B	624	LEU
1	B	625	MET
1	B	663	ASP
1	B	916	LEU
1	B	962	ARG
1	B	965	ASP
1	B	966	ILE
1	B	1031	ILE
1	B	1207	MET
1	C	45	ILE
1	C	137	LEU
1	C	138	MET
1	C	150	LEU
1	C	250	THR

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Mol	Chain	Res	Type
1	C	320	ASP
1	C	324	VAL
1	C	382	LEU
1	C	464	ASP
1	C	470	LYS
1	C	471	LEU
1	C	473	ILE
1	C	475	ASN
1	C	477	VAL
1	C	619	MET
1	C	625	MET
1	C	626	LYS
1	C	706	LEU
1	C	707	LYS
1	C	745	ARG
1	C	746	MET
1	C	863	LEU
1	C	873	LYS
1	C	962	ARG
1	C	1127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	343	HIS
1	A	657	HIS
1	A	662	ASN
1	A	942	GLN
1	A	1132	HIS
1	A	1171	HIS
1	D	343	HIS
1	D	446	GLN
1	D	846	ASN
1	D	1171	HIS
1	D	1176	GLN
1	B	118	ASN
1	B	432	ASN
1	B	525	ASN
1	B	689	GLN
1	B	693	GLN
1	B	711	ASN

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Mol	Chain	Res	Type
1	B	955	ASN
1	B	1092	ASN
1	B	1138	GLN
1	B	1139	HIS
1	C	43	HIS
1	C	63	HIS
1	C	258	HIS
1	C	309	ASN
1	C	403	GLN
1	C	424	GLN
1	C	446	GLN
1	C	480	HIS
1	C	525	ASN
1	C	675	ASN
1	C	689	GLN
1	C	693	GLN
1	C	696	GLN
1	C	1039	GLN
1	C	1092	ASN
1	C	1118	HIS
1	C	1132	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

28 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
2	Y01	B	1402	-	38,38,38	0.42	0	57,57,57	0.57	0
2	Y01	D	1403	-	38,38,38	0.42	0	57,57,57	0.58	1 (1%)
2	Y01	B	1405	-	38,38,38	0.37	0	57,57,57	0.44	0
2	Y01	D	1405	-	38,38,38	0.41	0	57,57,57	0.48	0
2	Y01	C	1402	-	38,38,38	0.38	0	57,57,57	0.45	0
2	Y01	A	1404	-	38,38,38	0.42	0	57,57,57	0.47	0
2	Y01	C	1403	-	38,38,38	0.44	0	57,57,57	0.62	1 (1%)
2	Y01	D	1401	-	38,38,38	0.35	0	57,57,57	0.42	0
2	Y01	D	1404	-	38,38,38	0.35	0	57,57,57	0.44	0
2	Y01	A	1401	-	38,38,38	0.36	0	57,57,57	0.45	0
2	Y01	C	1401	-	38,38,38	0.34	0	57,57,57	0.42	0
2	Y01	C	1405	-	38,38,38	0.37	0	57,57,57	0.43	0
3	A1AIA	D	1407	-	17,17,17	0.18	0	24,24,24	0.17	0
3	A1AIA	B	1406	-	17,17,17	0.17	0	24,24,24	0.18	0
2	Y01	B	1401	-	38,38,38	0.37	0	57,57,57	0.46	0
2	Y01	D	1406	-	38,38,38	0.37	0	57,57,57	0.46	0
2	Y01	A	1407	-	38,38,38	0.35	0	57,57,57	0.43	0
2	Y01	B	1403	-	38,38,38	0.35	0	57,57,57	0.44	0
2	Y01	A	1402	-	38,38,38	0.42	0	57,57,57	0.57	0
2	Y01	B	1404	-	38,38,38	0.41	0	57,57,57	0.47	0
2	Y01	C	1404	-	38,38,38	0.41	0	57,57,57	0.52	0
3	A1AIA	A	1406	-	17,17,17	0.16	0	24,24,24	0.18	0
2	Y01	B	1407	-	38,38,38	0.37	0	57,57,57	0.45	0
2	Y01	B	1408	-	38,38,38	0.40	0	57,57,57	0.47	0
2	Y01	D	1402	-	38,38,38	0.36	0	57,57,57	0.47	0
2	Y01	A	1405	-	38,38,38	0.37	0	57,57,57	0.44	0
2	Y01	A	1403	-	38,38,38	0.36	0	57,57,57	0.45	0
3	A1AIA	C	1406	-	17,17,17	0.18	0	24,24,24	0.24	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	Y01	B	1402	-	-	4/19/77/77	0/4/4/4
2	Y01	D	1403	-	-	4/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	B	1405	-	-	10/19/77/77	0/4/4/4
2	Y01	D	1405	-	-	5/19/77/77	0/4/4/4
2	Y01	C	1402	-	-	8/19/77/77	0/4/4/4
2	Y01	A	1404	-	-	6/19/77/77	0/4/4/4
2	Y01	C	1403	-	-	10/19/77/77	0/4/4/4
2	Y01	D	1401	-	-	7/19/77/77	0/4/4/4
2	Y01	D	1404	-	-	14/19/77/77	0/4/4/4
2	Y01	A	1401	-	-	8/19/77/77	0/4/4/4
2	Y01	C	1401	-	-	6/19/77/77	0/4/4/4
2	Y01	C	1405	-	-	10/19/77/77	0/4/4/4
3	A1AIA	D	1407	-	-	0/9/27/27	0/2/2/2
3	A1AIA	B	1406	-	-	0/9/27/27	0/2/2/2
2	Y01	B	1401	-	-	8/19/77/77	0/4/4/4
2	Y01	D	1406	-	-	10/19/77/77	0/4/4/4
2	Y01	A	1407	-	-	8/19/77/77	0/4/4/4
2	Y01	B	1403	-	-	13/19/77/77	0/4/4/4
2	Y01	A	1402	-	-	4/19/77/77	0/4/4/4
2	Y01	B	1404	-	-	5/19/77/77	0/4/4/4
2	Y01	C	1404	-	-	5/19/77/77	0/4/4/4
3	A1AIA	A	1406	-	-	1/9/27/27	0/2/2/2
2	Y01	B	1407	-	-	4/19/77/77	0/4/4/4
2	Y01	B	1408	-	-	10/19/77/77	0/4/4/4
2	Y01	D	1402	-	-	8/19/77/77	0/4/4/4
2	Y01	A	1405	-	-	10/19/77/77	0/4/4/4
2	Y01	A	1403	-	-	10/19/77/77	0/4/4/4
3	A1AIA	C	1406	-	-	0/9/27/27	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1403	Y01	CAP-CAQ-CBG	-2.77	99.72	105.14
2	D	1403	Y01	CAP-CAQ-CBG	-2.04	101.14	105.14

There are no chirality outliers.

All (188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1405	Y01	CAC-CBB-CBE-CAP
2	A	1405	Y01	CAC-CBB-CBE-CBI
2	D	1406	Y01	CAC-CBB-CBE-CAP
2	D	1406	Y01	CAC-CBB-CBE-CBI
2	B	1405	Y01	CAC-CBB-CBE-CAP
2	B	1405	Y01	CAC-CBB-CBE-CBI
2	B	1407	Y01	CAJ-CAO-CBB-CAC
2	D	1404	Y01	CAC-CBB-CBE-CAP
2	B	1403	Y01	CAC-CBB-CBE-CAP
2	A	1403	Y01	CAC-CBB-CBE-CBI
2	D	1404	Y01	CAC-CBB-CBE-CBI
2	B	1403	Y01	CAC-CBB-CBE-CBI
2	A	1405	Y01	CAO-CBB-CBE-CBI
2	D	1406	Y01	CAO-CBB-CBE-CBI
2	B	1405	Y01	CAO-CBB-CBE-CBI
2	A	1403	Y01	CAJ-CAO-CBB-CAC
2	A	1405	Y01	CAJ-CAO-CBB-CAC
2	D	1404	Y01	CAJ-CAO-CBB-CAC
2	D	1406	Y01	CAJ-CAO-CBB-CAC
2	B	1405	Y01	CAJ-CAO-CBB-CAC
2	C	1405	Y01	CAJ-CAO-CBB-CAC
2	A	1403	Y01	CAC-CBB-CBE-CAP
2	A	1403	Y01	CAO-CBB-CBE-CAP
2	A	1405	Y01	CAO-CBB-CBE-CAP
2	D	1406	Y01	CAO-CBB-CBE-CAP
2	B	1405	Y01	CAO-CBB-CBE-CAP
2	A	1403	Y01	CAO-CBB-CBE-CBI
2	D	1404	Y01	CAO-CBB-CBE-CBI
2	B	1403	Y01	CAO-CBB-CBE-CBI
2	B	1408	Y01	CAO-CBB-CBE-CBI
2	A	1404	Y01	CAJ-CAO-CBB-CAC
2	B	1404	Y01	CAJ-CAO-CBB-CAC
2	D	1404	Y01	CAO-CBB-CBE-CAP
2	B	1403	Y01	CAO-CBB-CBE-CAP
2	A	1405	Y01	CAJ-CAO-CBB-CBE
2	A	1401	Y01	CAJ-CAO-CBB-CAC
2	D	1402	Y01	CAJ-CAO-CBB-CAC
2	D	1405	Y01	CAJ-CAO-CBB-CAC
2	B	1401	Y01	CAJ-CAO-CBB-CAC
2	B	1403	Y01	CAJ-CAO-CBB-CAC
2	C	1402	Y01	CAJ-CAO-CBB-CAC
2	C	1403	Y01	CAJ-CAO-CBB-CAC
2	D	1406	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
2	B	1405	Y01	CAJ-CAO-CBB-CBE
2	B	1408	Y01	CAJ-CAO-CBB-CBE
2	C	1405	Y01	CAJ-CAO-CBB-CBE
2	B	1408	Y01	CAC-CBB-CBE-CAP
2	A	1403	Y01	CAJ-CAO-CBB-CBE
2	D	1403	Y01	CAJ-CAO-CBB-CBE
2	D	1404	Y01	CAJ-CAO-CBB-CBE
2	A	1407	Y01	CAJ-CAO-CBB-CAC
2	D	1403	Y01	CAJ-CAO-CBB-CAC
2	A	1401	Y01	CAJ-CAO-CBB-CBE
2	A	1402	Y01	CAJ-CAO-CBB-CBE
2	D	1402	Y01	CAJ-CAO-CBB-CBE
2	B	1401	Y01	CAJ-CAO-CBB-CBE
2	B	1403	Y01	CAJ-CAO-CBB-CBE
2	C	1402	Y01	CAJ-CAO-CBB-CBE
2	B	1408	Y01	CAC-CBB-CBE-CBI
2	B	1408	Y01	CAO-CBB-CBE-CAP
2	B	1402	Y01	CAJ-CAO-CBB-CBE
2	D	1401	Y01	CAN-CAJ-CAO-CBB
2	A	1405	Y01	CAN-CAJ-CAO-CBB
2	D	1406	Y01	CAN-CAJ-CAO-CBB
2	B	1405	Y01	CAN-CAJ-CAO-CBB
2	B	1408	Y01	CAO-CAJ-CAN-CBA
2	C	1404	Y01	CAJ-CAO-CBB-CAC
2	C	1402	Y01	CAX-CAL-CAM-CAY
2	B	1407	Y01	CAO-CAJ-CAN-CBA
2	B	1407	Y01	CAN-CAJ-CAO-CBB
2	A	1402	Y01	CAJ-CAO-CBB-CAC
2	C	1401	Y01	CAJ-CAO-CBB-CAC
2	C	1403	Y01	CAX-CAL-CAM-CAY
2	C	1402	Y01	CAO-CAJ-CAN-CBA
2	C	1401	Y01	CAO-CBB-CBE-CBI
2	A	1407	Y01	CAN-CAJ-CAO-CBB
2	B	1402	Y01	CAJ-CAO-CBB-CAC
2	C	1405	Y01	CAO-CBB-CBE-CBI
2	D	1401	Y01	CAJ-CAO-CBB-CAC
2	A	1407	Y01	CAO-CBB-CBE-CBI
2	B	1408	Y01	CAJ-CAO-CBB-CAC
2	B	1408	Y01	CAJ-CAN-CBA-CAB
2	A	1404	Y01	CAN-CAJ-CAO-CBB
2	B	1404	Y01	CAN-CAJ-CAO-CBB
2	B	1404	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
2	A	1401	Y01	CAO-CBB-CBE-CBI
2	C	1405	Y01	CAN-CAJ-CAO-CBB
2	A	1404	Y01	CAO-CAJ-CAN-CBA
2	D	1405	Y01	CAN-CAJ-CAO-CBB
2	D	1405	Y01	CAO-CAJ-CAN-CBA
2	A	1407	Y01	CAC-CBB-CBE-CAP
2	C	1401	Y01	CAC-CBB-CBE-CAP
2	C	1405	Y01	CAC-CBB-CBE-CAP
2	C	1401	Y01	CAC-CBB-CBE-CBI
2	A	1407	Y01	CAC-CBB-CBE-CBI
2	C	1405	Y01	CAC-CBB-CBE-CBI
2	C	1401	Y01	CAO-CBB-CBE-CAP
2	C	1405	Y01	CAO-CBB-CBE-CAP
2	C	1404	Y01	CAO-CAJ-CAN-CBA
2	B	1401	Y01	CAO-CBB-CBE-CBI
2	A	1407	Y01	CAO-CBB-CBE-CAP
2	C	1401	Y01	CAN-CAJ-CAO-CBB
2	A	1401	Y01	CAO-CBB-CBE-CAP
2	B	1401	Y01	CAO-CBB-CBE-CAP
2	D	1401	Y01	CAO-CBB-CBE-CBI
2	D	1402	Y01	CAO-CBB-CBE-CBI
2	D	1401	Y01	CAC-CBB-CBE-CAP
2	D	1401	Y01	CAO-CBB-CBE-CAP
2	D	1402	Y01	CAO-CBB-CBE-CAP
2	D	1401	Y01	CAO-CAJ-CAN-CBA
2	B	1408	Y01	CAJ-CAN-CBA-CAA
2	A	1401	Y01	CAC-CBB-CBE-CBI
2	D	1401	Y01	CAC-CBB-CBE-CBI
2	B	1403	Y01	CAO-CAJ-CAN-CBA
2	A	1401	Y01	CAC-CBB-CBE-CAP
2	C	1403	Y01	CAO-CBB-CBE-CAP
2	B	1401	Y01	CAC-CBB-CBE-CBI
2	D	1402	Y01	CAC-CBB-CBE-CBI
2	C	1404	Y01	CAN-CAJ-CAO-CBB
2	B	1407	Y01	CAJ-CAO-CBB-CBE
2	C	1403	Y01	CAO-CBB-CBE-CBI
2	C	1402	Y01	CAO-CBB-CBE-CAP
2	B	1401	Y01	CAC-CBB-CBE-CAP
2	D	1402	Y01	CAC-CBB-CBE-CAP
2	C	1403	Y01	CAC-CBB-CBE-CAP
2	D	1404	Y01	CAJ-CAN-CBA-CAB
2	C	1403	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
2	C	1403	Y01	CAM-CAL-CAX-OAF
2	A	1403	Y01	CAM-CAL-CAX-OAF
2	D	1406	Y01	CAO-CAJ-CAN-CBA
2	A	1402	Y01	CAM-CAL-CAX-OAF
2	C	1403	Y01	CAM-CAL-CAX-OAH
2	D	1406	Y01	CAM-CAL-CAX-OAF
2	B	1405	Y01	CAM-CAL-CAX-OAF
2	C	1402	Y01	CAO-CBB-CBE-CBI
2	D	1402	Y01	CAM-CAL-CAX-OAH
2	D	1402	Y01	CAM-CAL-CAX-OAF
2	D	1404	Y01	CAM-CAL-CAX-OAF
2	B	1403	Y01	CAM-CAL-CAX-OAF
2	A	1402	Y01	CAM-CAL-CAX-OAH
2	A	1403	Y01	CAM-CAL-CAX-OAH
2	D	1403	Y01	CAM-CAL-CAX-OAF
2	B	1402	Y01	CAM-CAL-CAX-OAH
2	D	1403	Y01	CAM-CAL-CAX-OAH
2	A	1405	Y01	CAM-CAL-CAX-OAF
2	B	1402	Y01	CAM-CAL-CAX-OAF
2	D	1404	Y01	CAJ-CAN-CBA-CAA
2	C	1404	Y01	CAM-CAL-CAX-OAF
2	C	1405	Y01	CAM-CAL-CAX-OAF
2	B	1405	Y01	CAO-CAJ-CAN-CBA
2	A	1405	Y01	CAO-CAJ-CAN-CBA
2	C	1405	Y01	CAM-CAL-CAX-OAH
2	B	1401	Y01	CAM-CAL-CAX-OAH
2	B	1403	Y01	CAM-CAL-CAX-OAH
2	A	1405	Y01	CAM-CAL-CAX-OAH
2	D	1404	Y01	CAM-CAL-CAX-OAH
2	D	1406	Y01	CAM-CAL-CAX-OAH
2	B	1405	Y01	CAM-CAL-CAX-OAH
2	A	1401	Y01	CAM-CAL-CAX-OAH
2	B	1403	Y01	CAJ-CAN-CBA-CAB
2	C	1404	Y01	CAM-CAL-CAX-OAH
2	A	1401	Y01	CAM-CAL-CAX-OAF
2	B	1401	Y01	CAM-CAL-CAX-OAF
2	D	1404	Y01	CAO-CAJ-CAN-CBA
2	C	1403	Y01	CAL-CAM-CAY-OAW
2	C	1402	Y01	CAM-CAL-CAX-OAH
2	C	1402	Y01	CAM-CAL-CAX-OAF
2	B	1403	Y01	CAL-CAM-CAY-OAW
2	B	1403	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
2	D	1404	Y01	CAX-CAL-CAM-CAY
3	A	1406	A1AIA	C01-C02-C03-C09
2	A	1403	Y01	CAL-CAM-CAY-OAW
2	A	1407	Y01	CAM-CAL-CAX-OAH
2	D	1404	Y01	CAL-CAM-CAY-OAW
2	B	1408	Y01	CAL-CAM-CAY-OAW
2	A	1404	Y01	CAM-CAL-CAX-OAF
2	C	1405	Y01	CAO-CAJ-CAN-CBA
2	B	1403	Y01	CAL-CAM-CAY-OAG
2	B	1404	Y01	CAM-CAL-CAX-OAF
2	A	1403	Y01	CAL-CAM-CAY-OAG
2	C	1403	Y01	CAL-CAM-CAY-OAG
2	B	1404	Y01	CAL-CAM-CAY-OAW
2	D	1405	Y01	CAL-CAM-CAY-OAW
2	D	1404	Y01	CAL-CAM-CAY-OAG
2	A	1407	Y01	CAM-CAL-CAX-OAF
2	A	1404	Y01	CAL-CAM-CAY-OAW
2	A	1404	Y01	CAM-CAL-CAX-OAH
2	D	1405	Y01	CAM-CAL-CAX-OAF

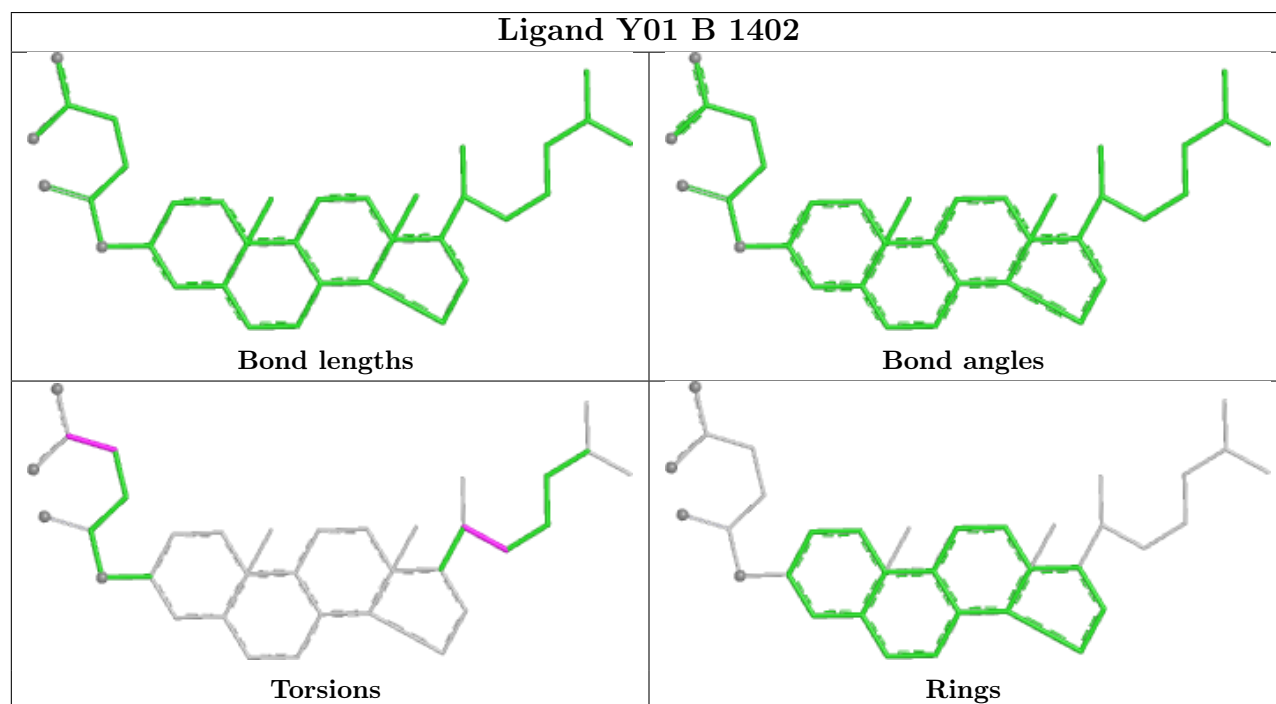
There are no ring outliers.

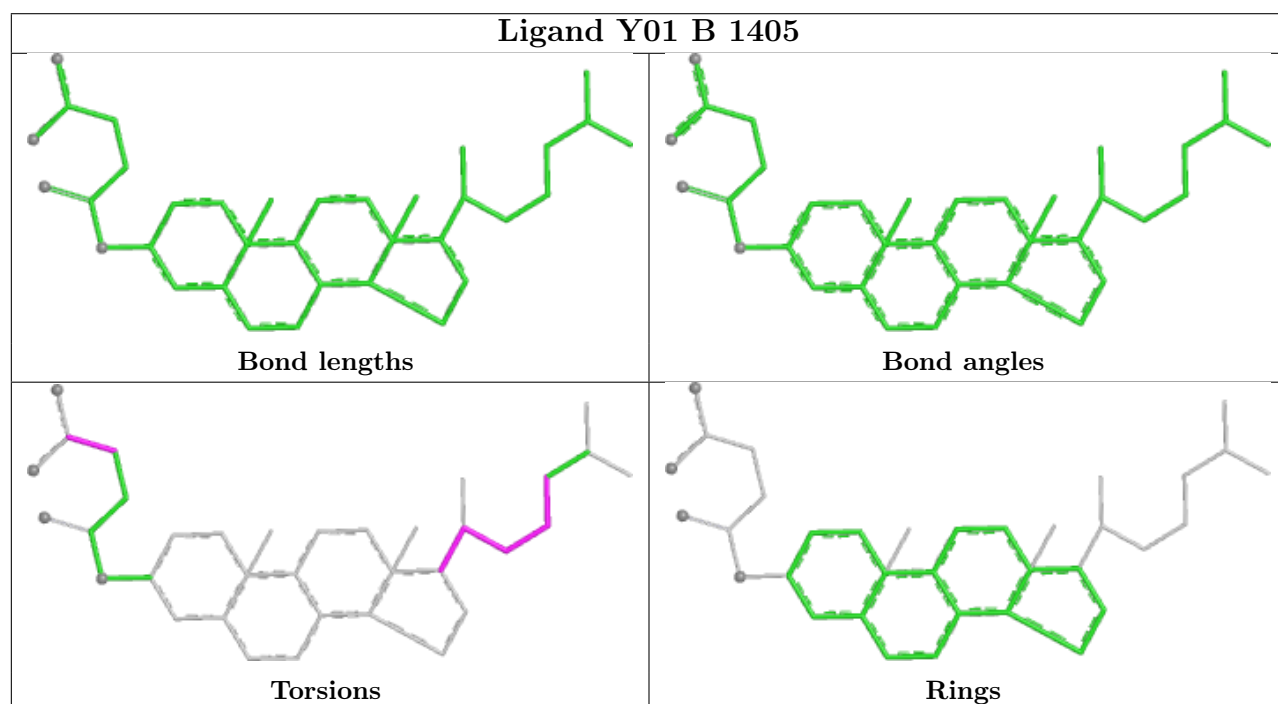
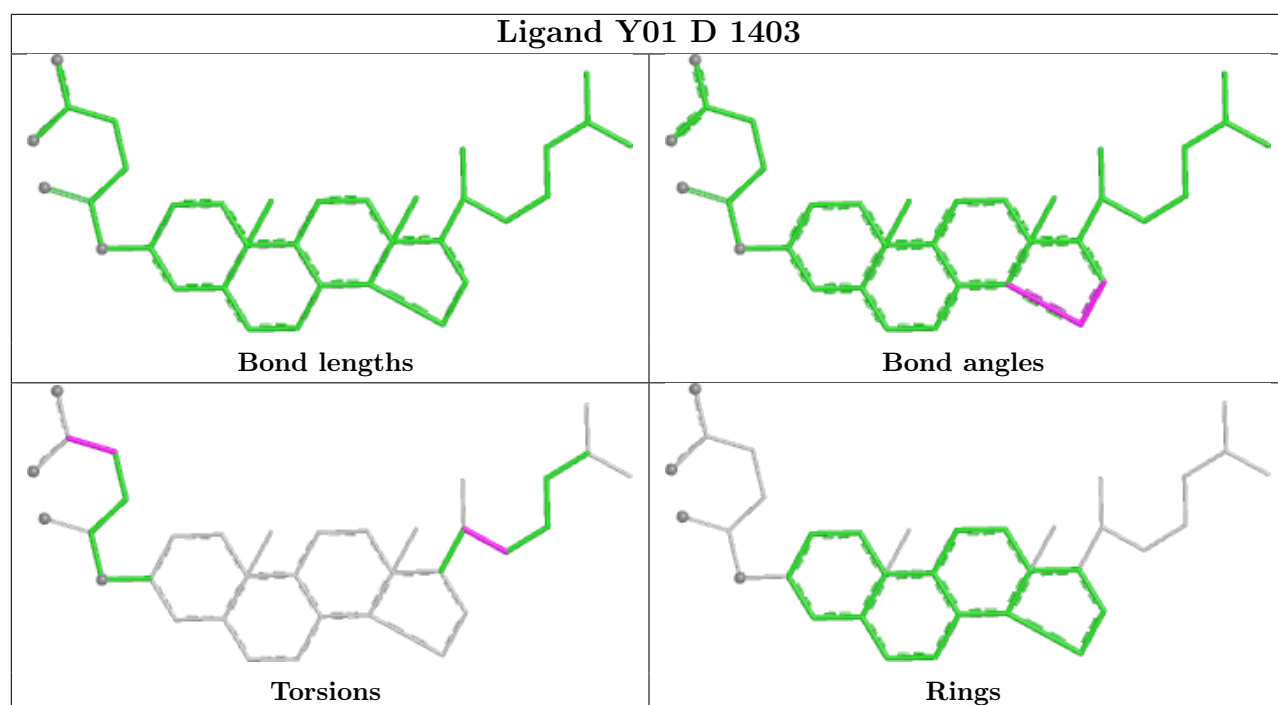
16 monomers are involved in 23 short contacts:

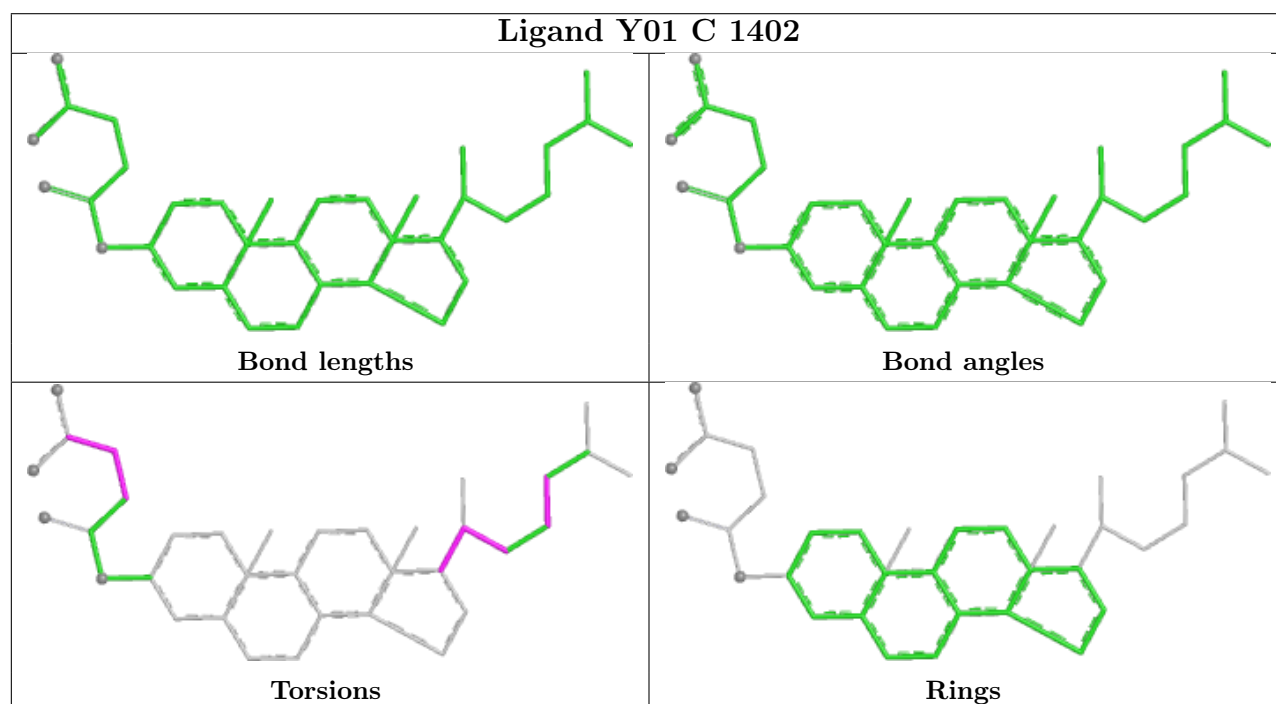
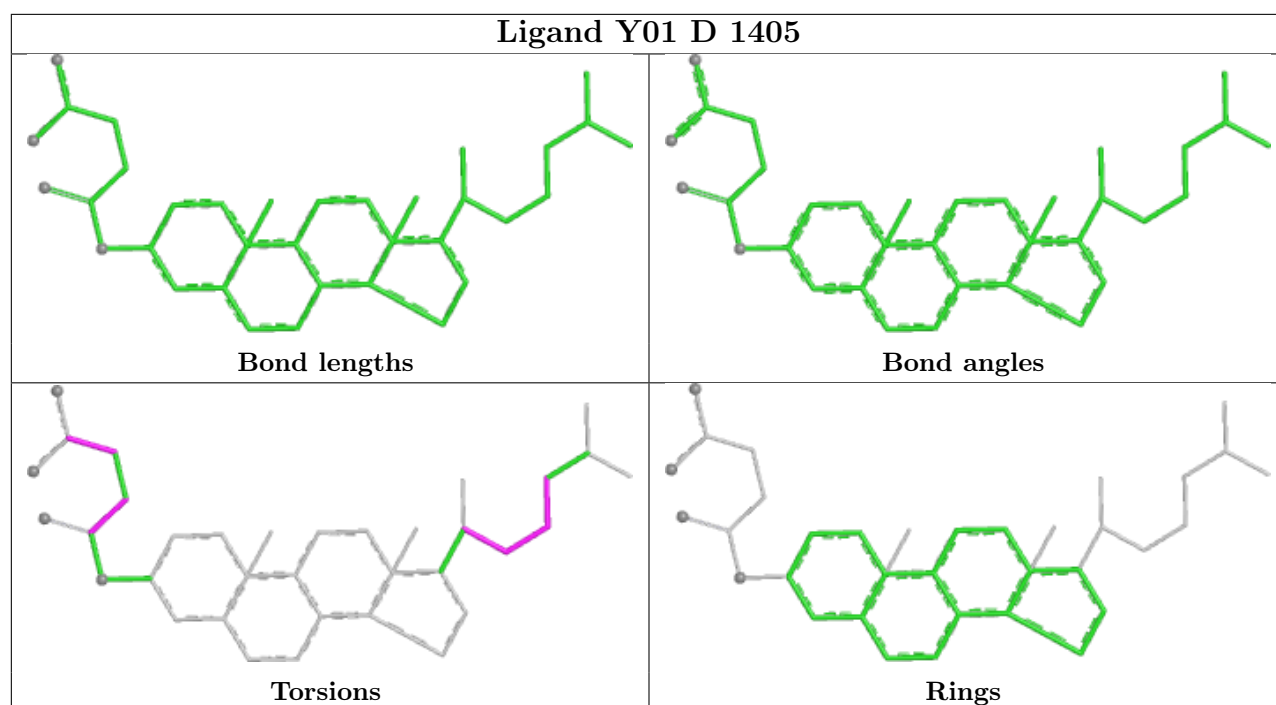
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1405	Y01	3	0
2	D	1405	Y01	2	0
2	C	1403	Y01	1	0
2	D	1401	Y01	1	0
2	D	1404	Y01	1	0
2	C	1401	Y01	1	0
2	C	1405	Y01	2	0
2	B	1401	Y01	1	0
2	D	1406	Y01	2	0
2	A	1407	Y01	1	0
2	B	1403	Y01	2	0
2	A	1402	Y01	1	0
2	B	1407	Y01	1	0
2	B	1408	Y01	2	0
2	A	1405	Y01	1	0
2	A	1403	Y01	1	0

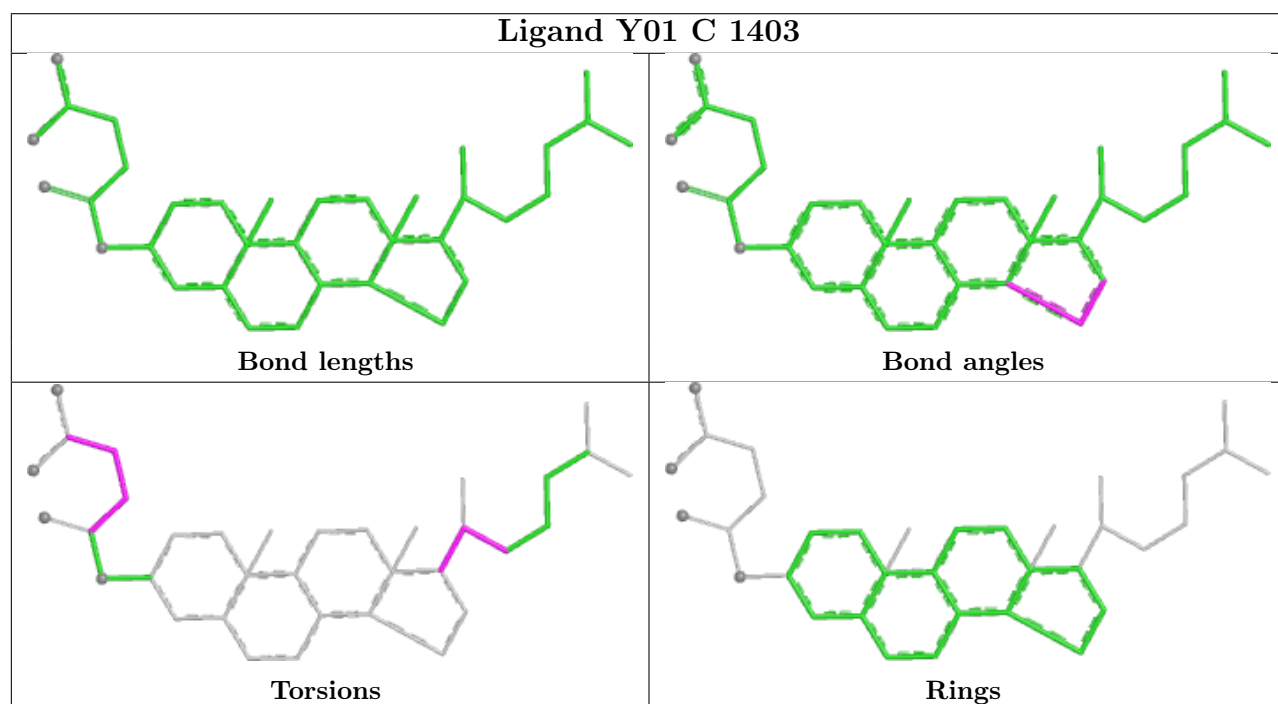
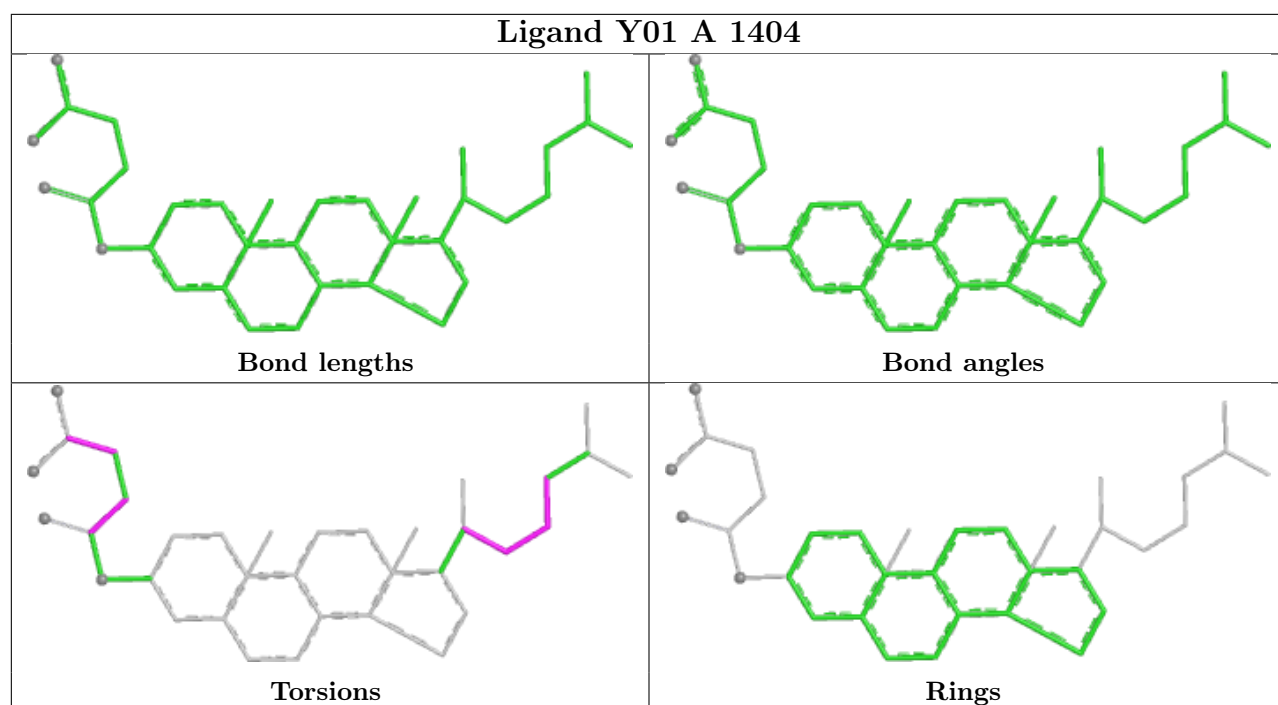
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

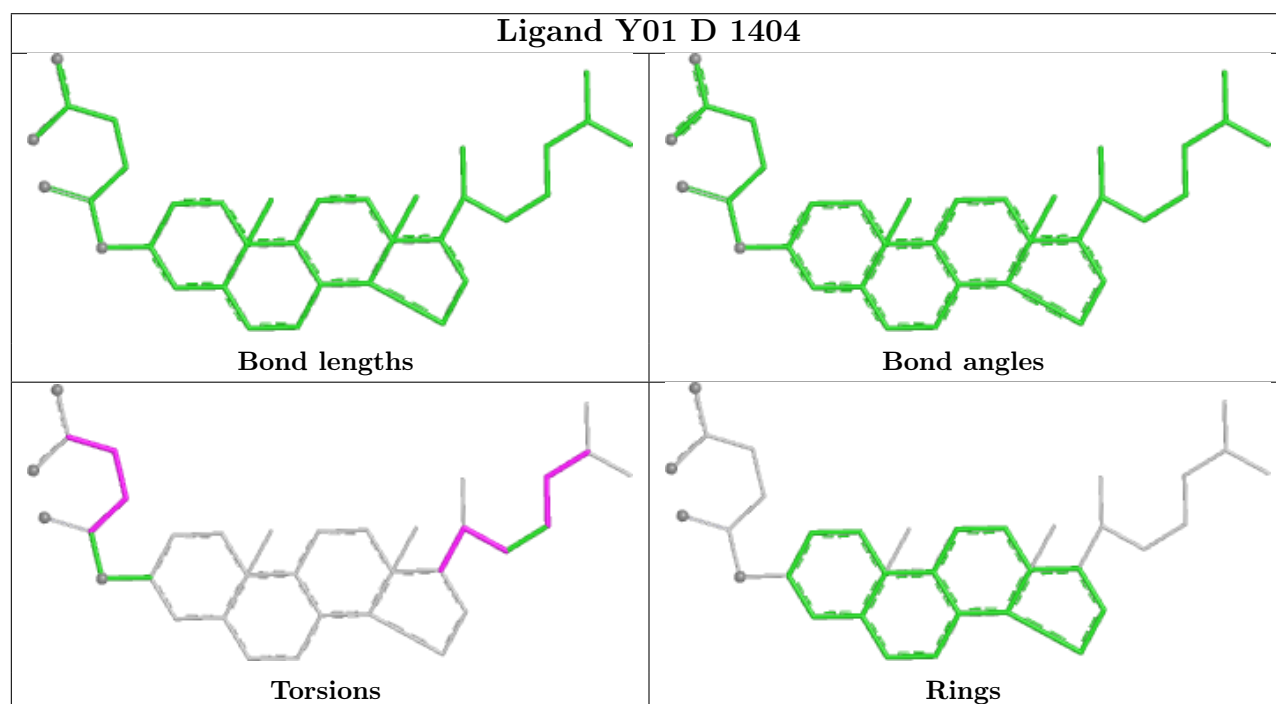
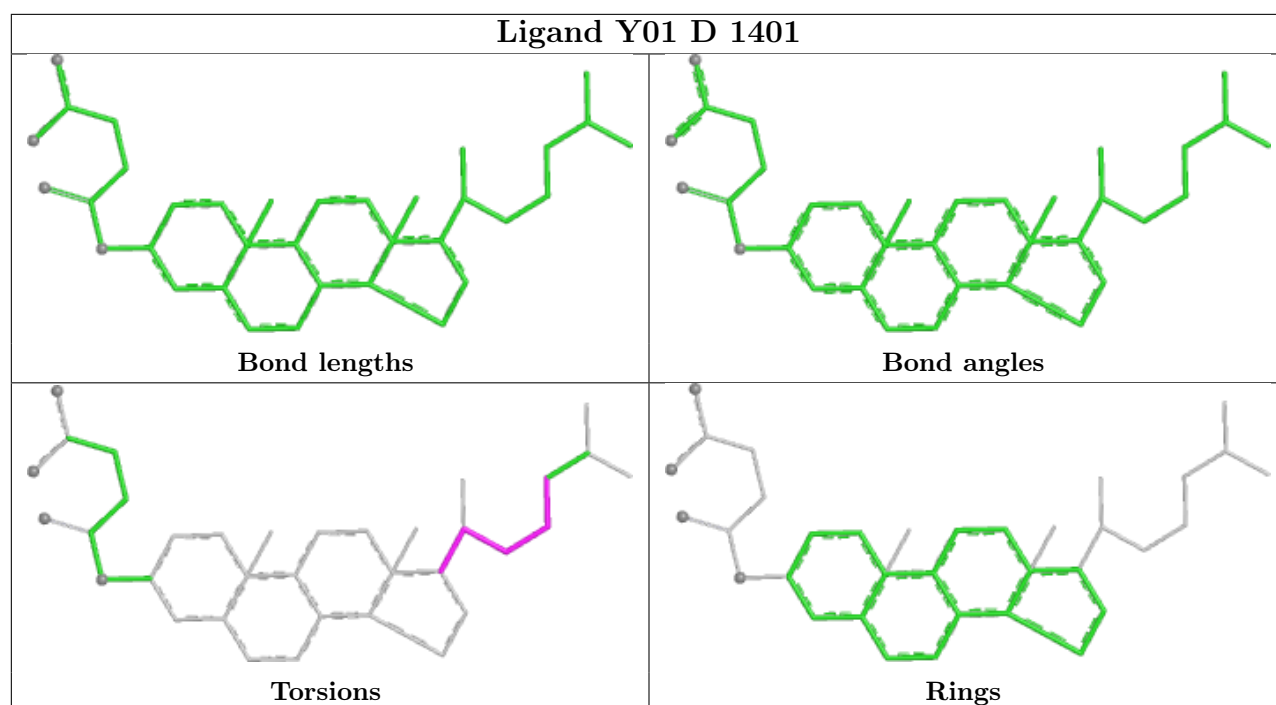


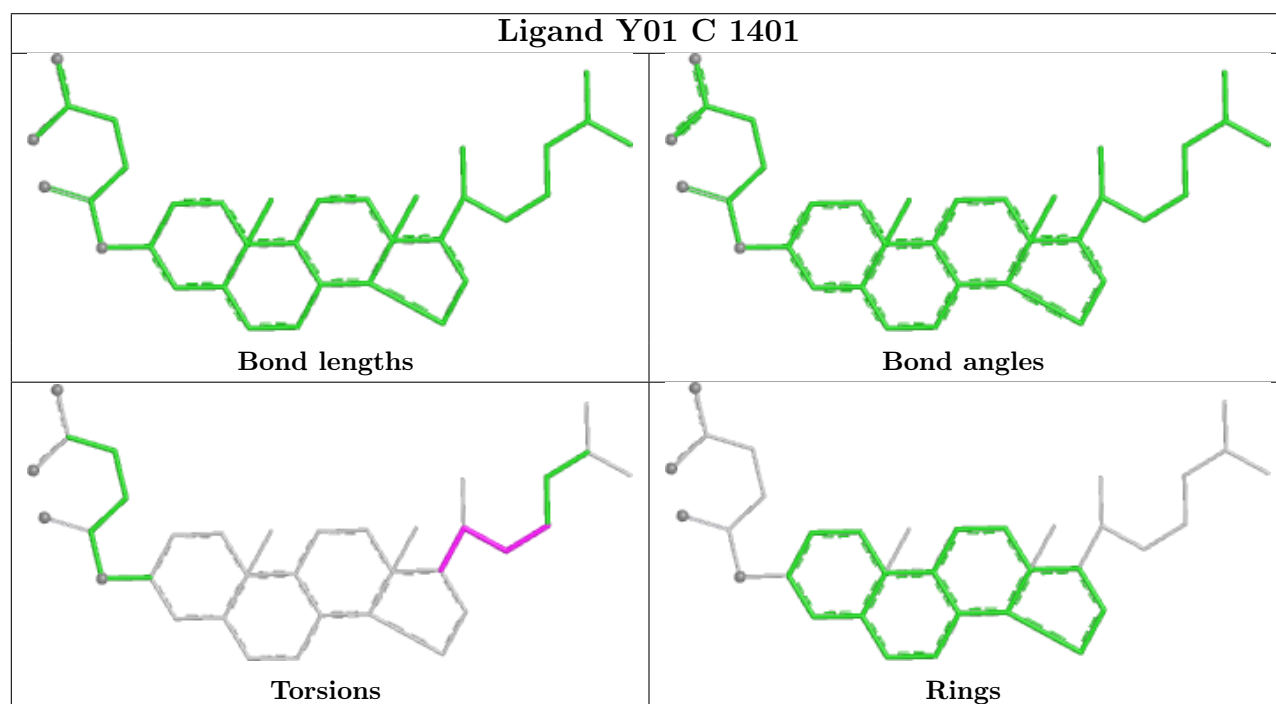
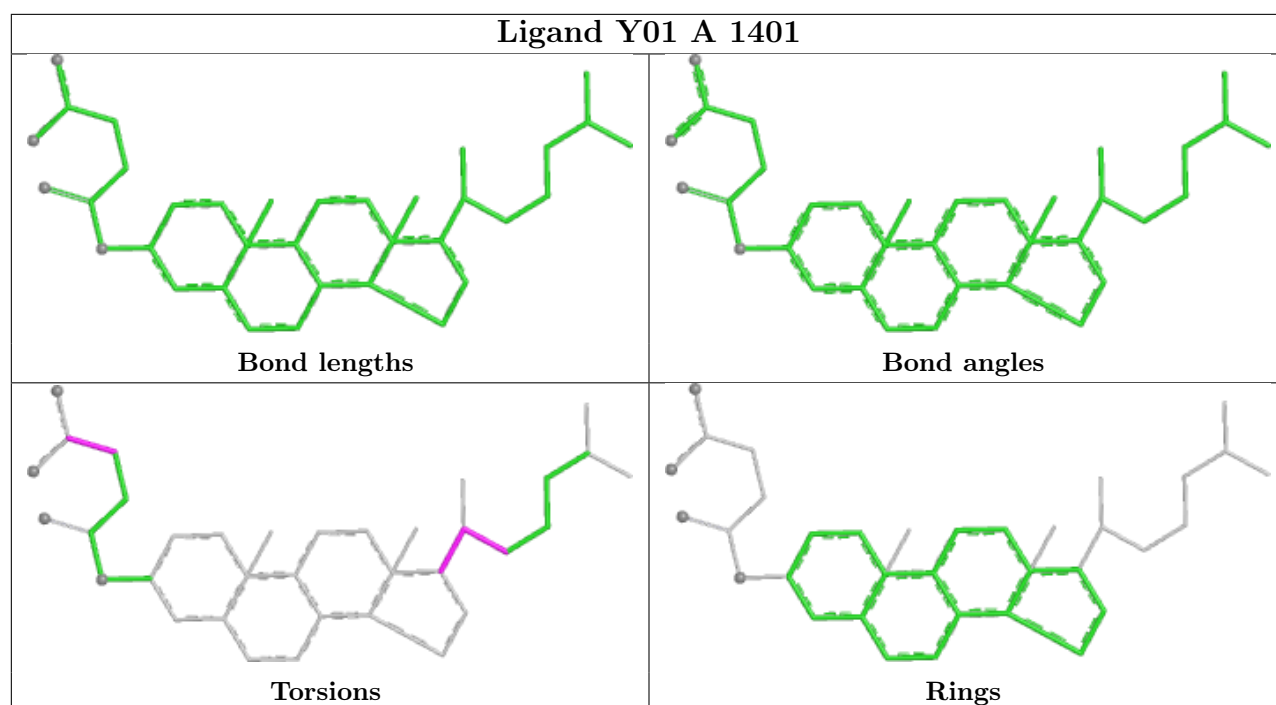


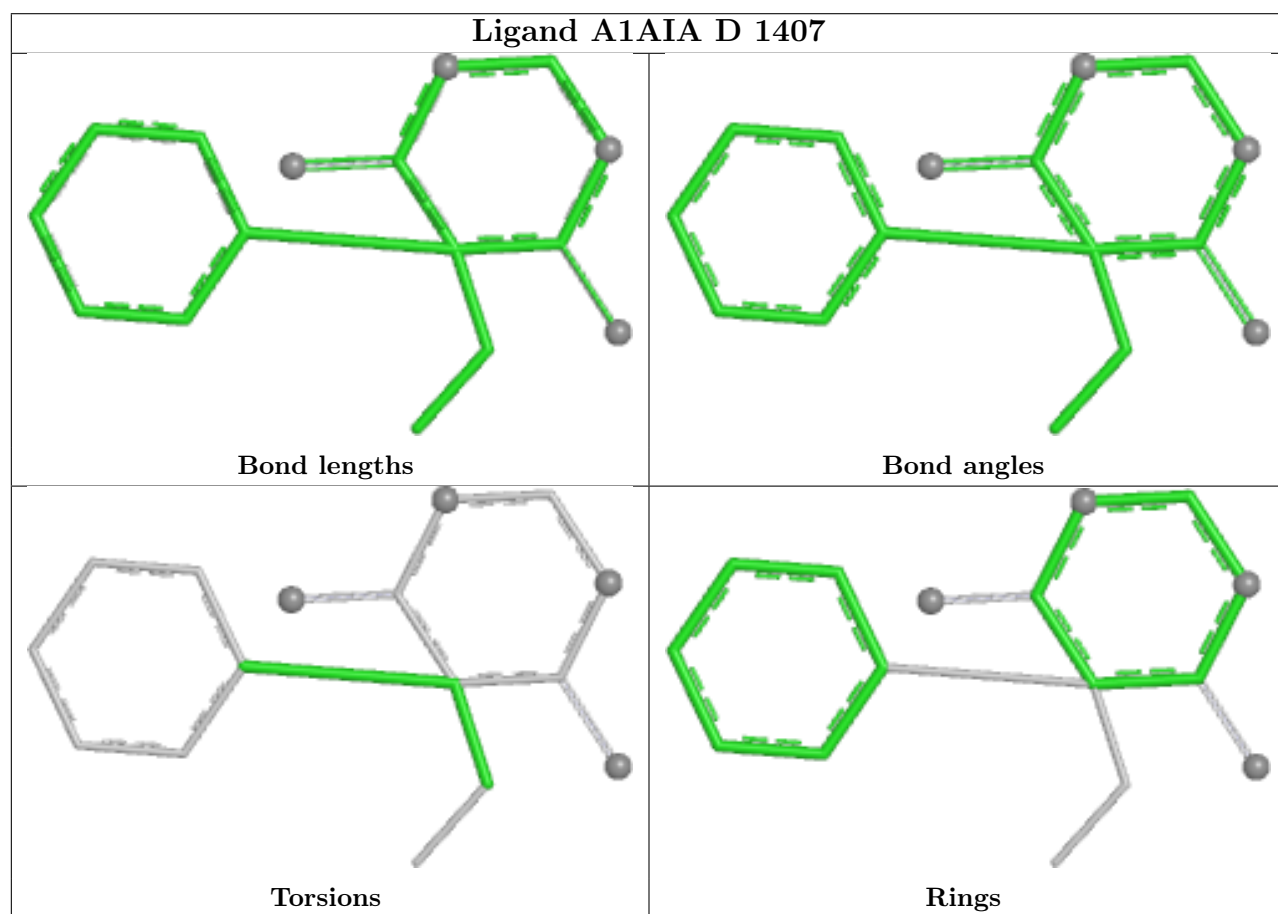
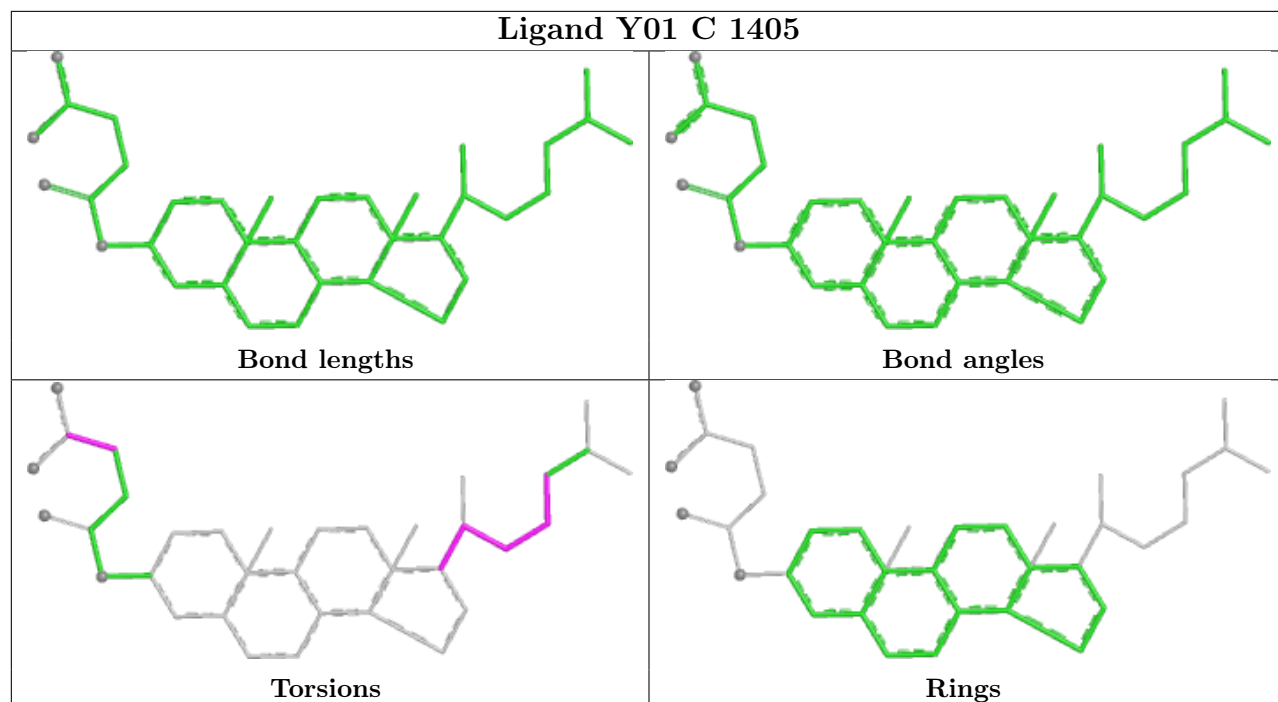


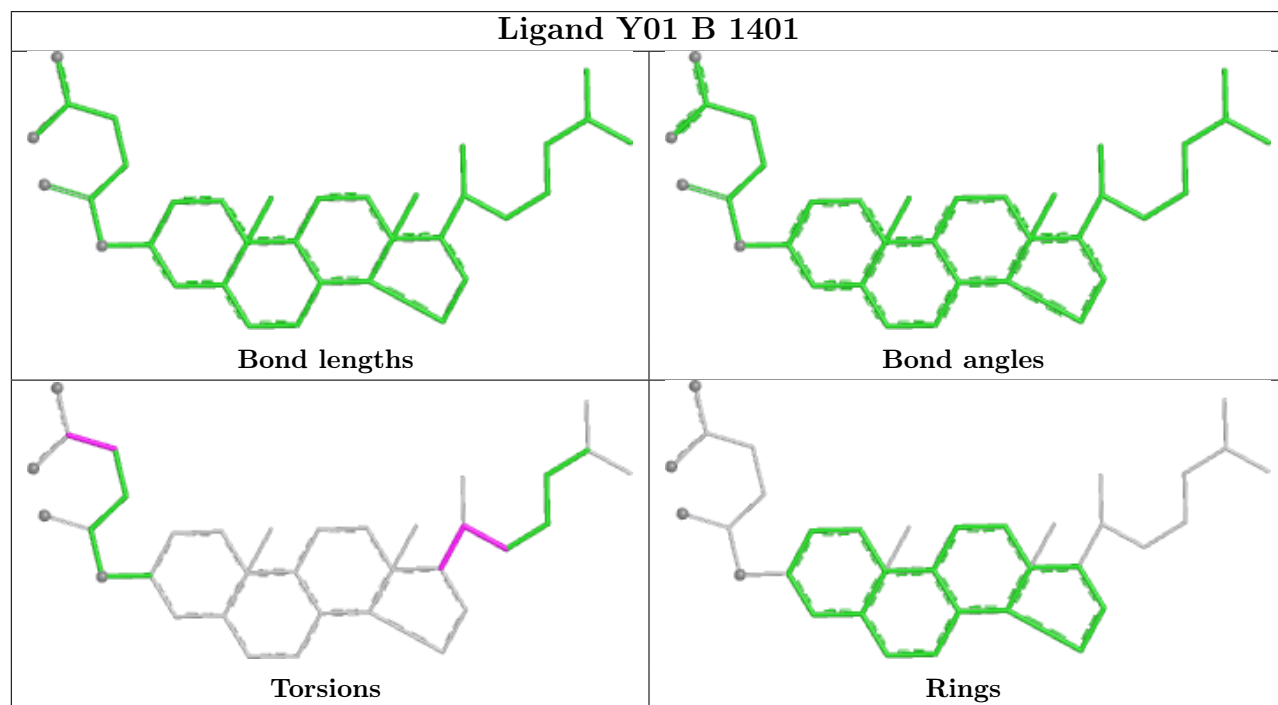
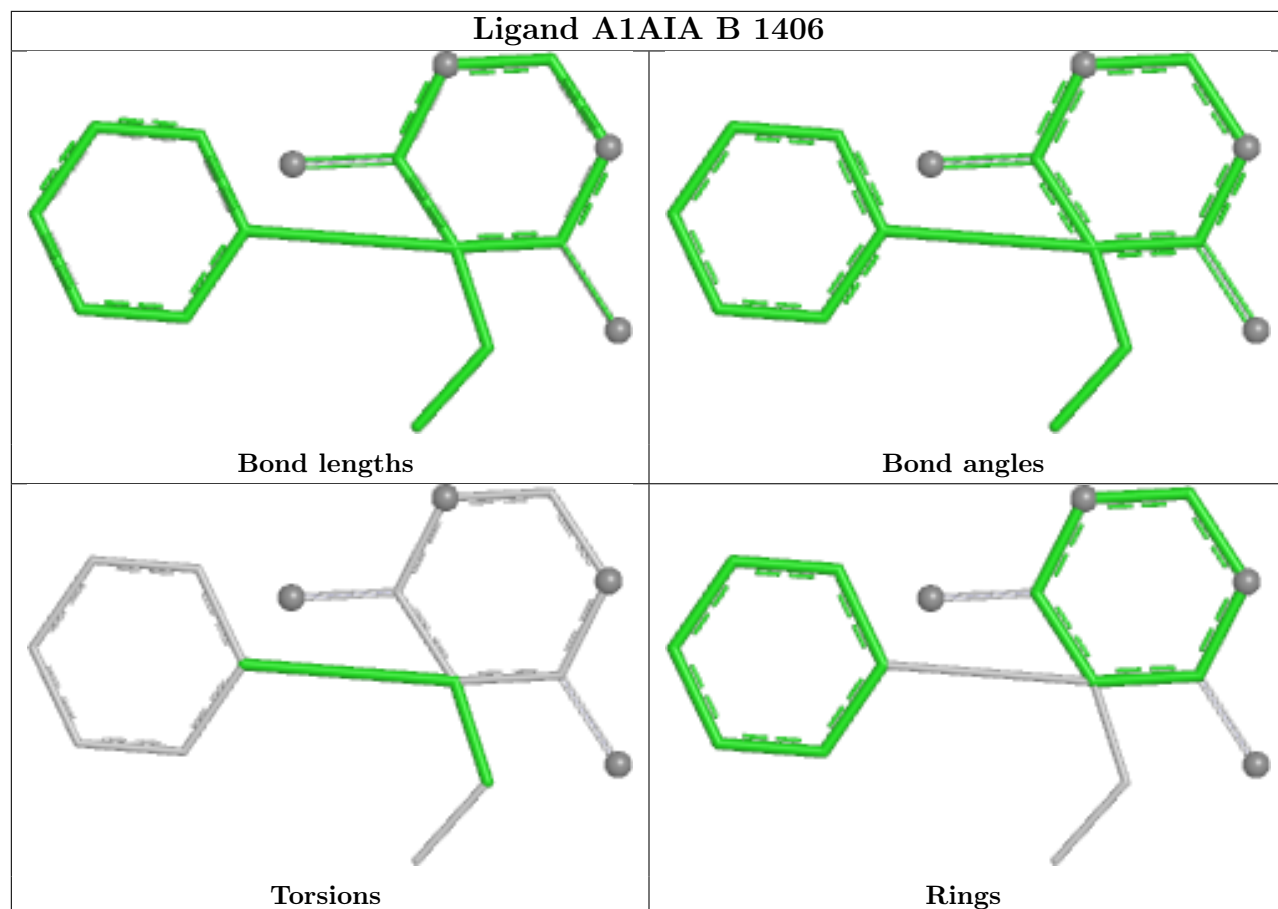


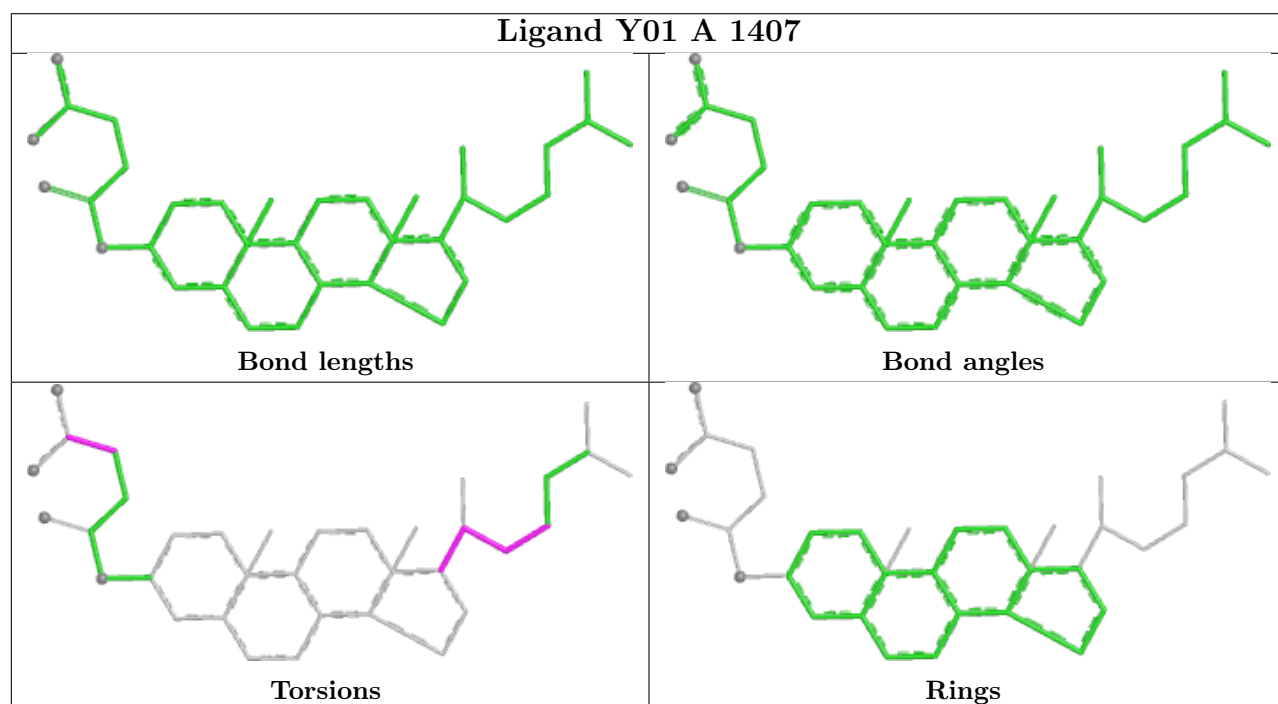
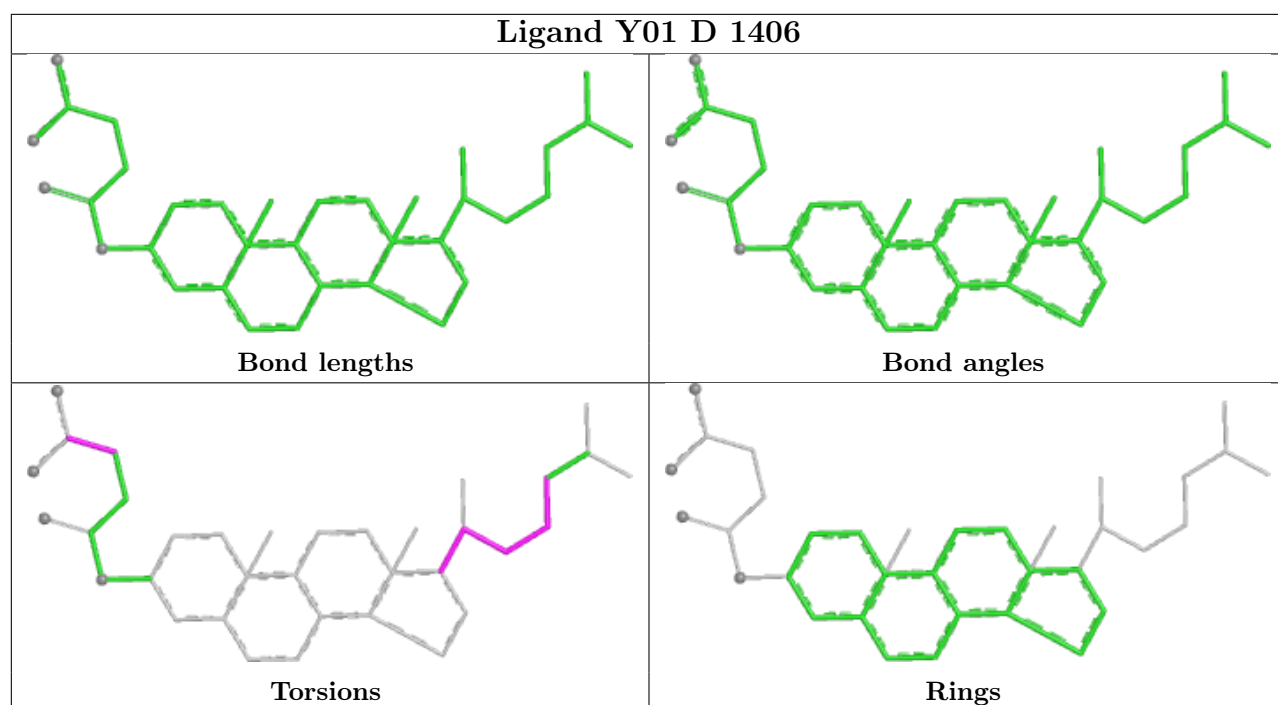


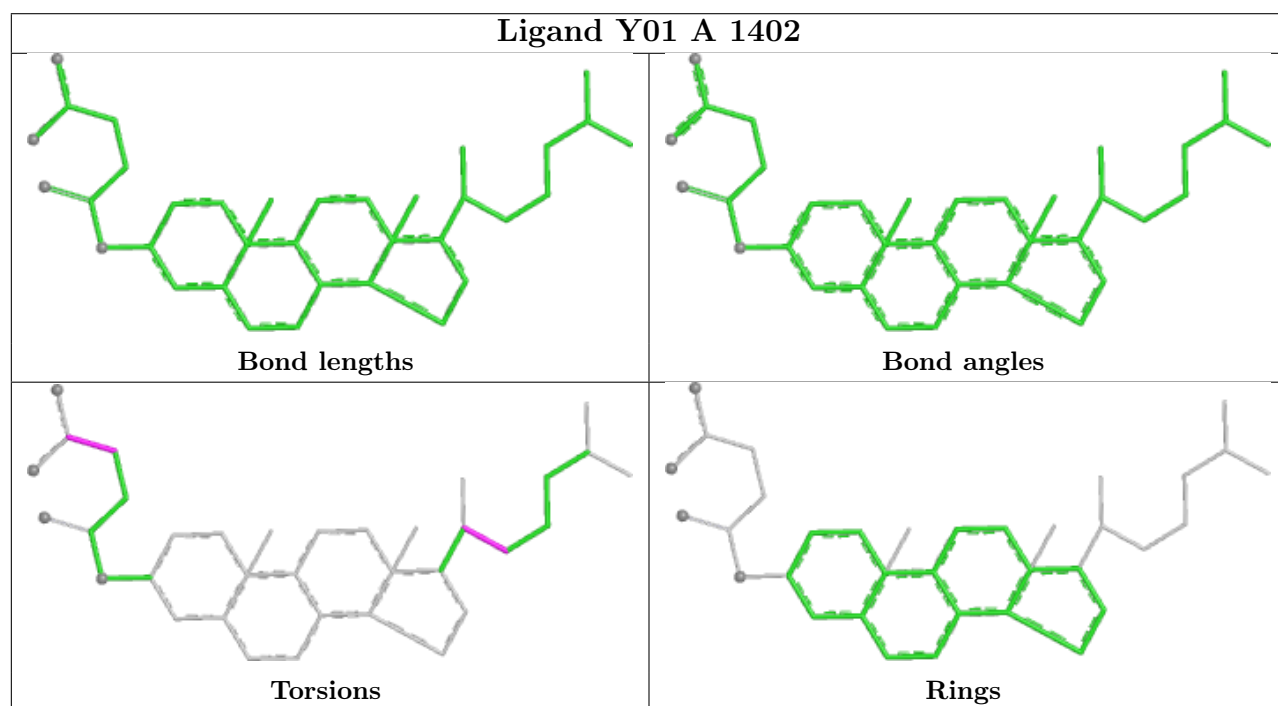
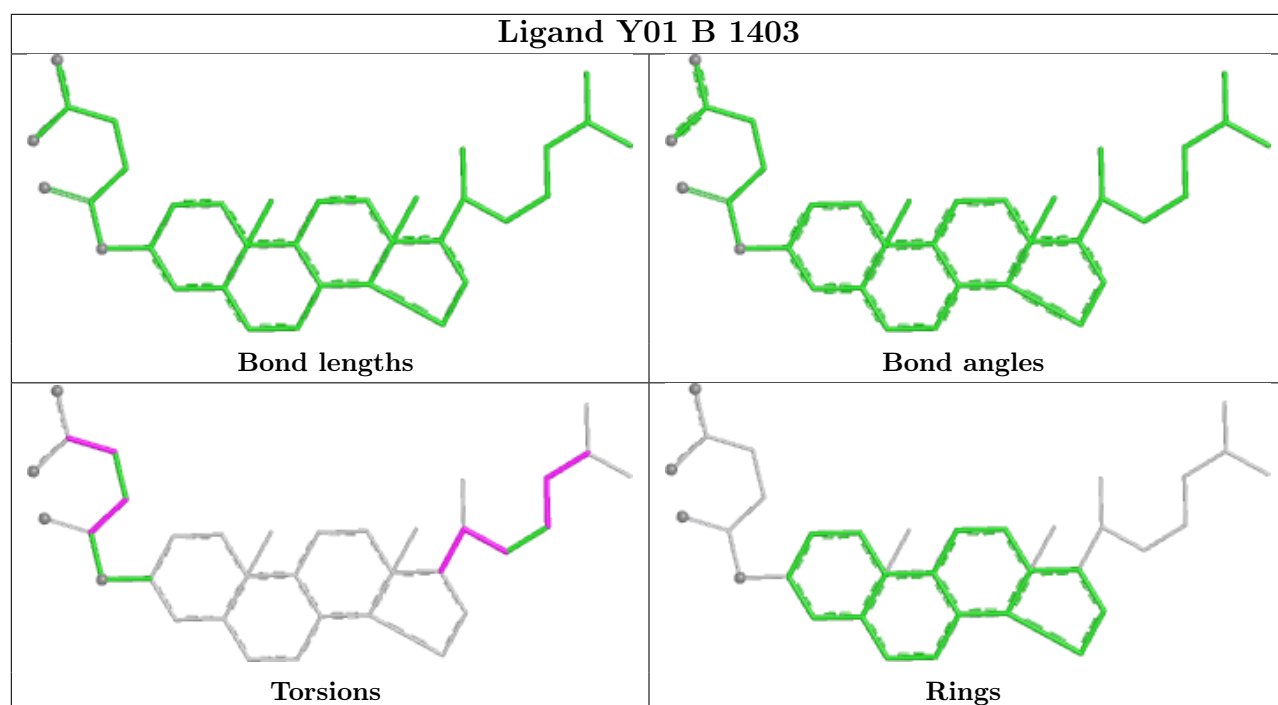


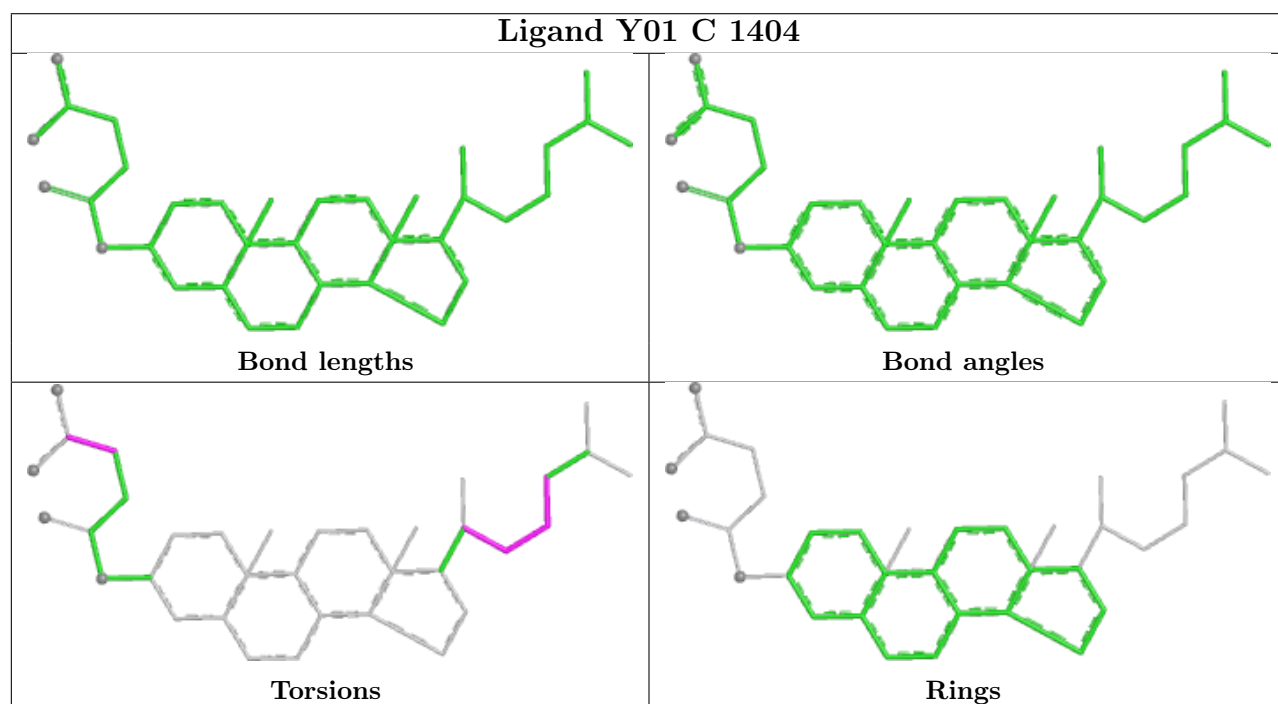
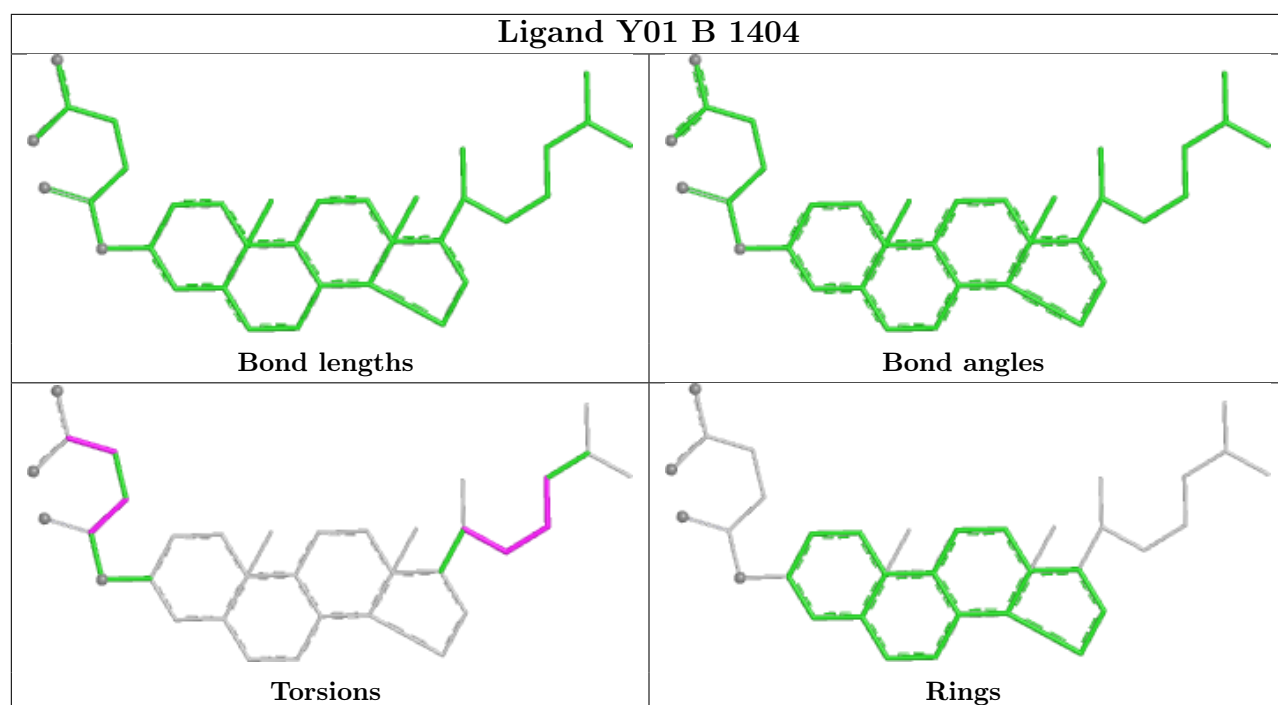


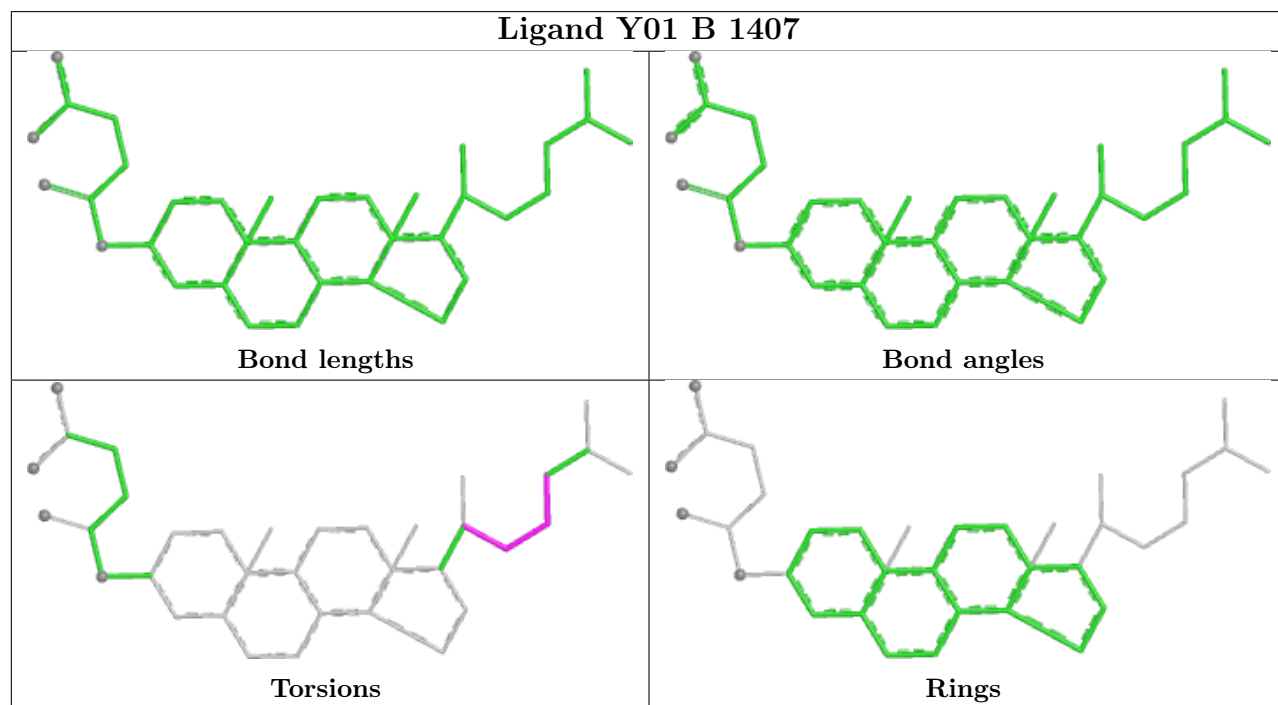
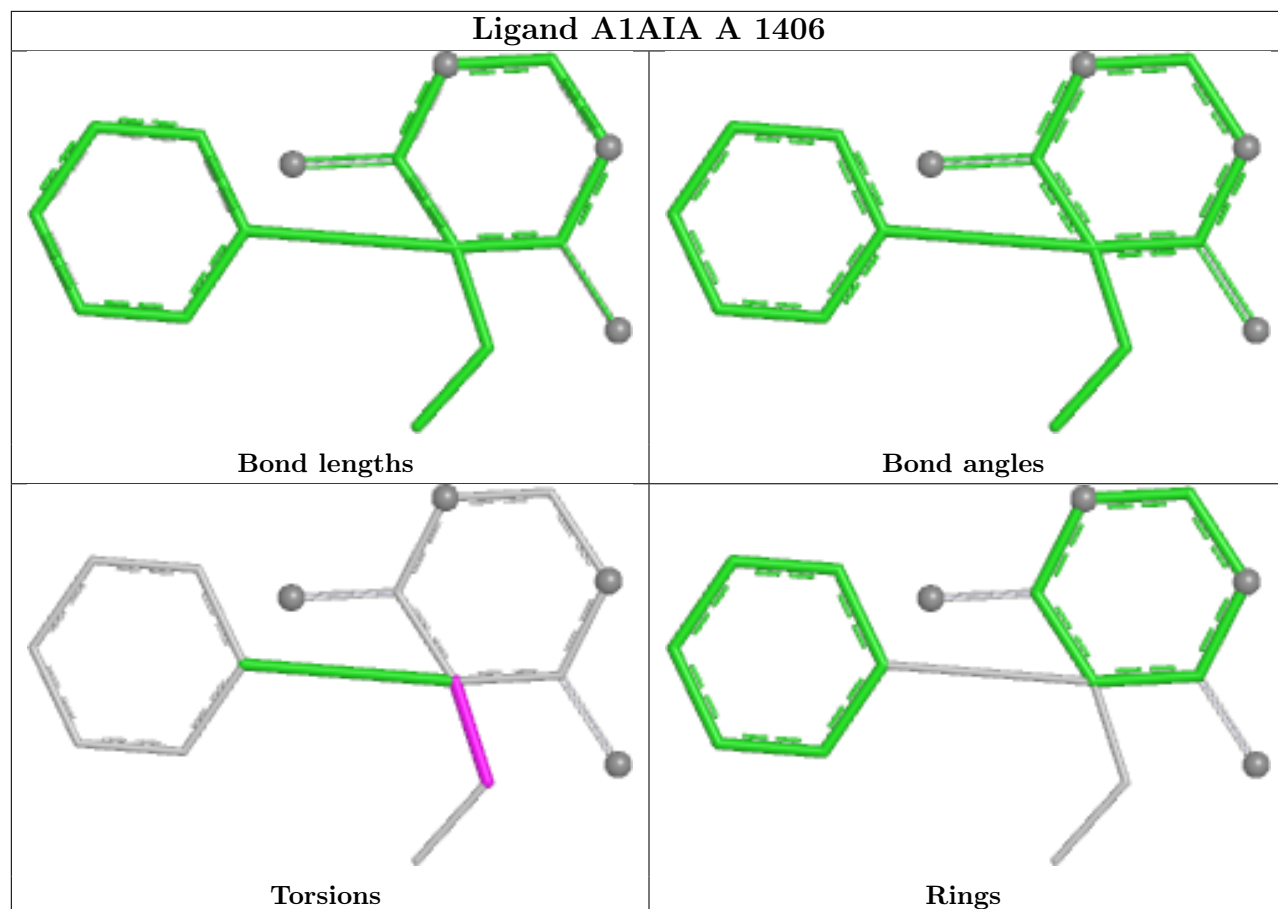




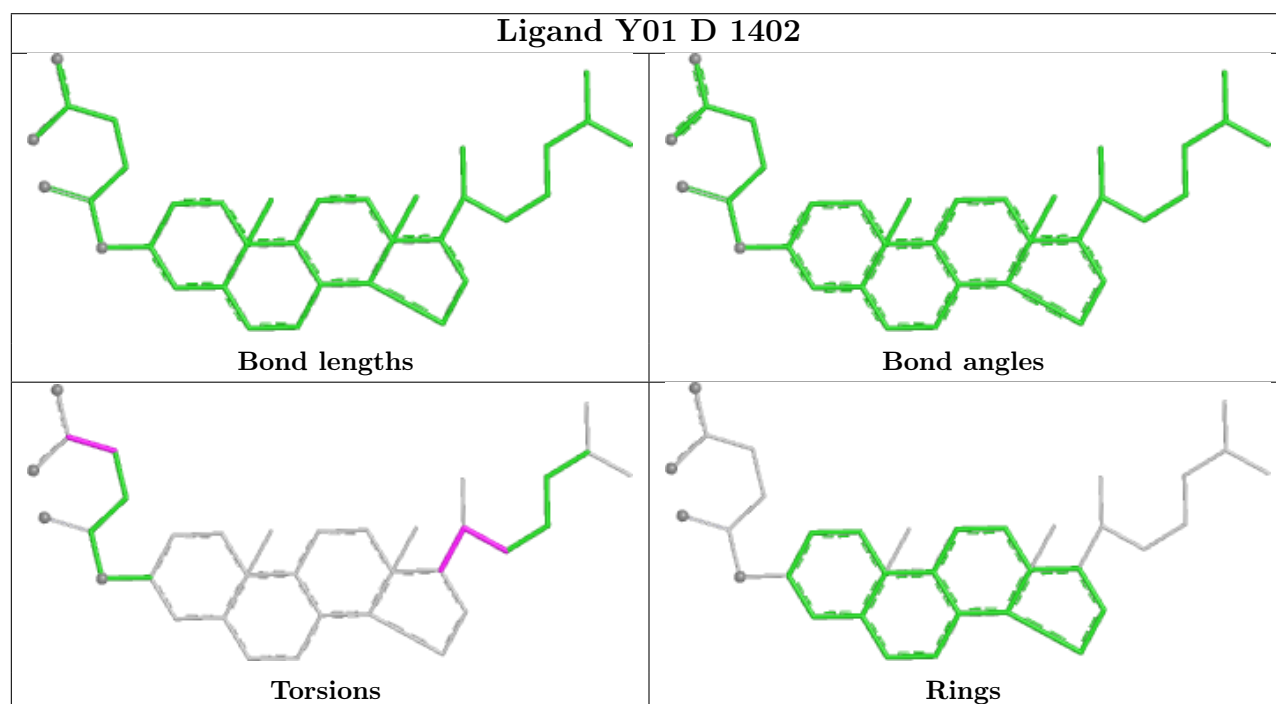
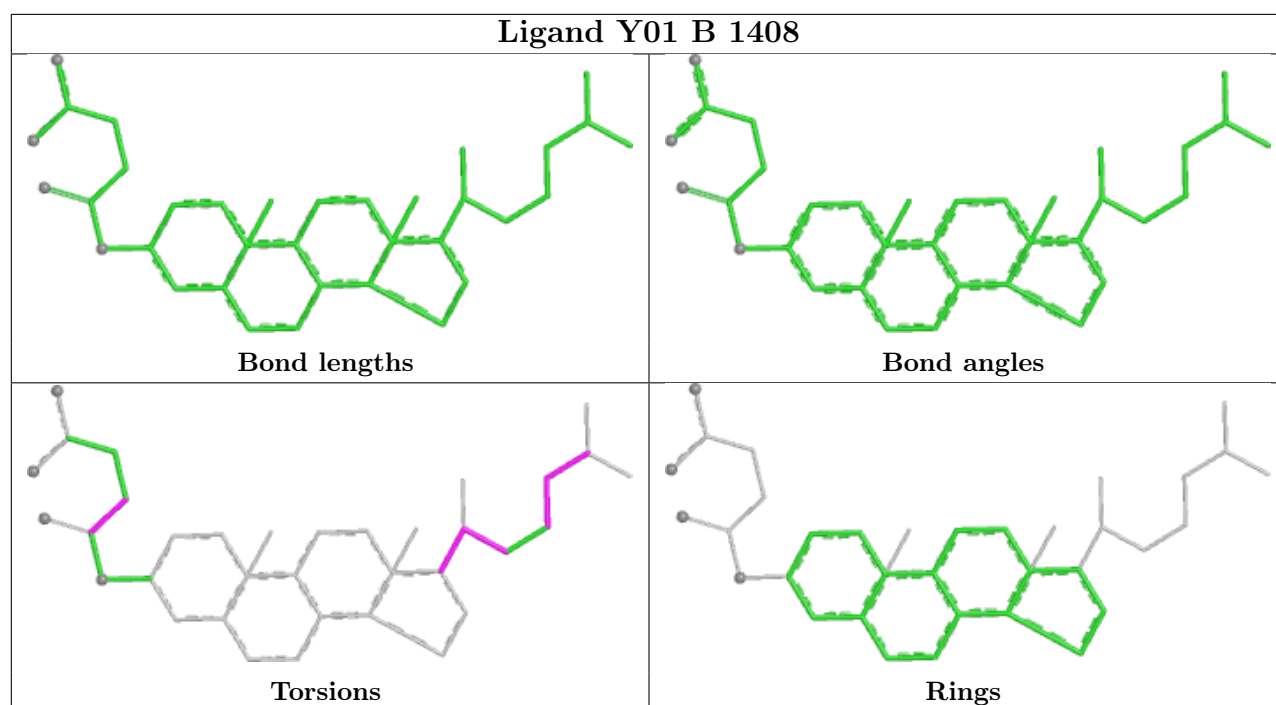


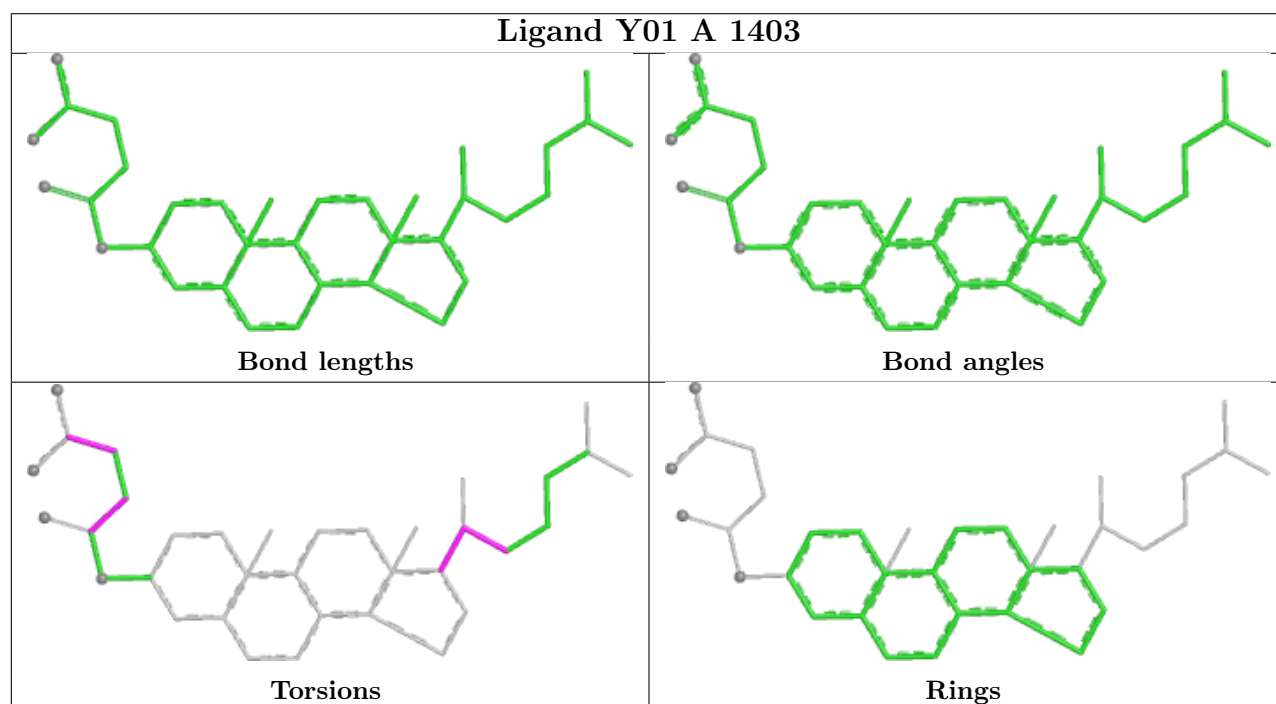
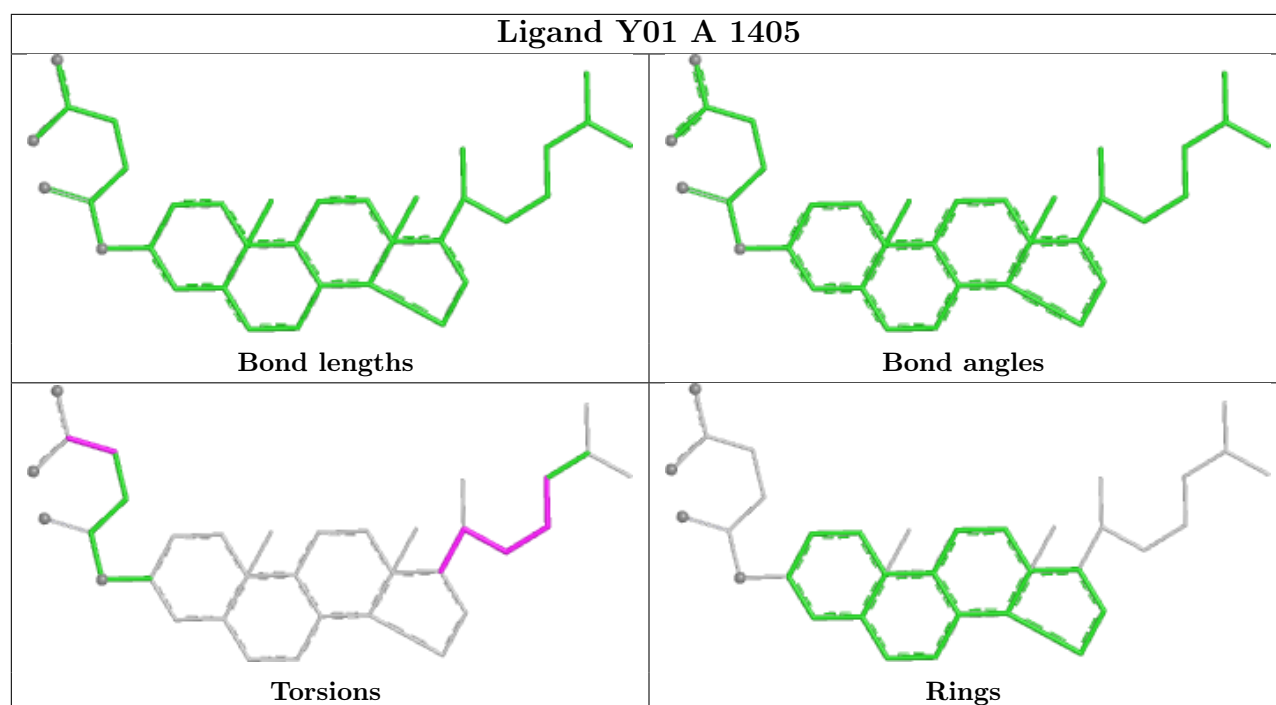


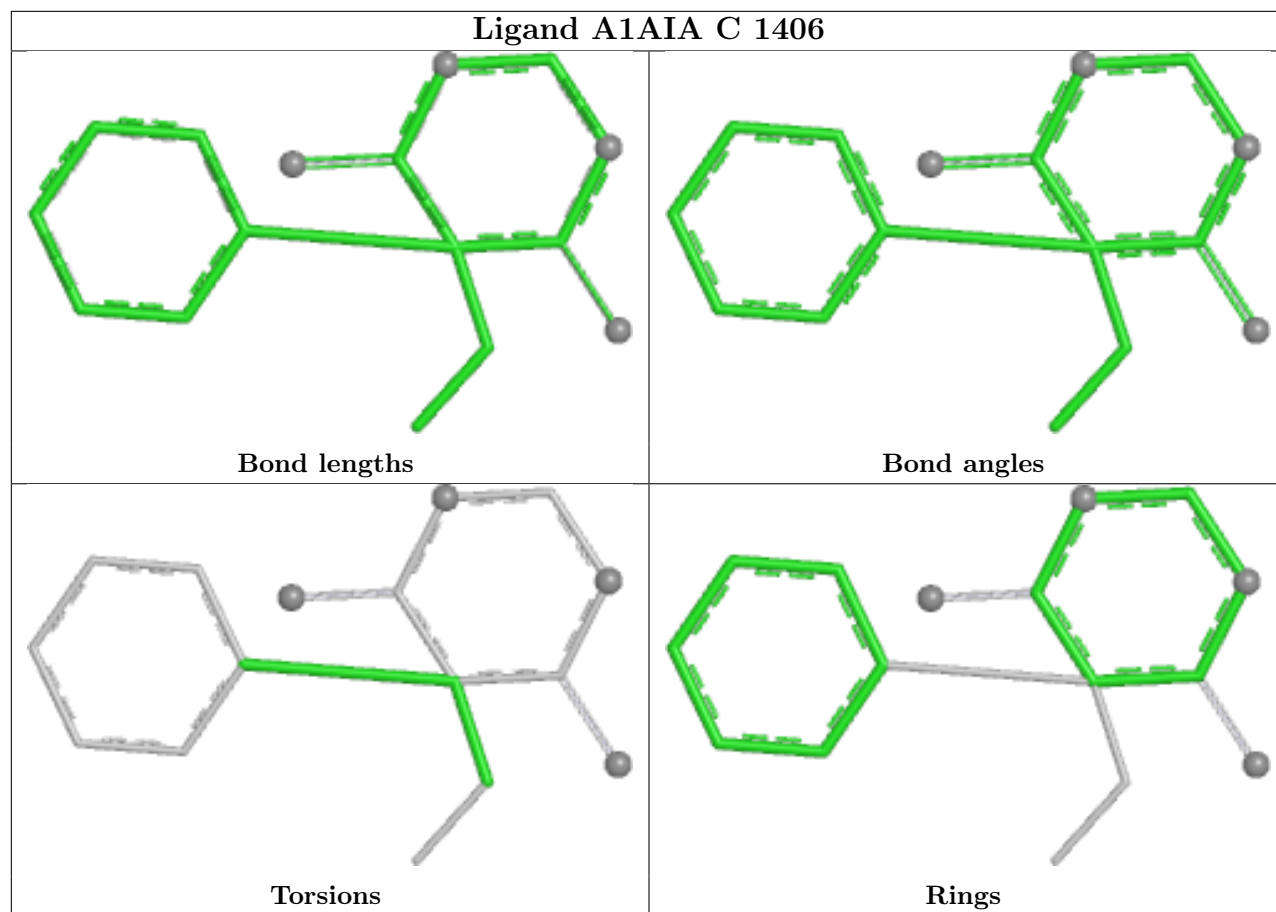












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

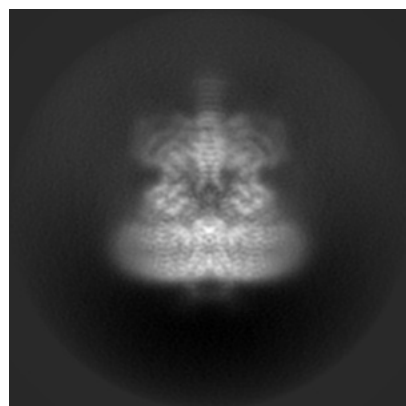
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70226. These allow visual inspection of the internal detail of the map and identification of artifacts.

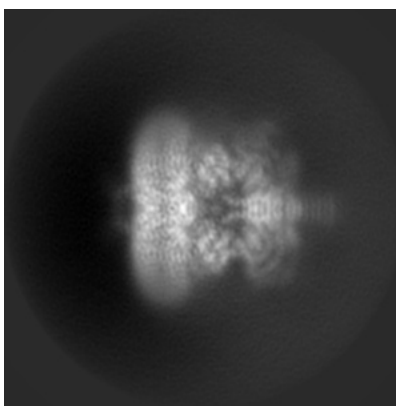
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

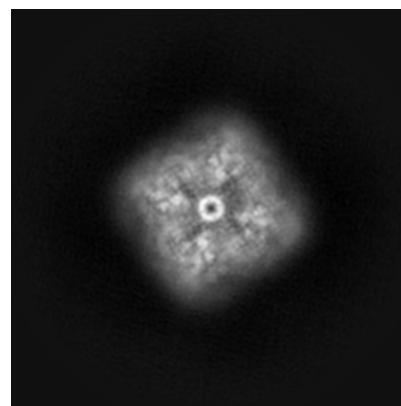
#### 6.1.1 Primary map



X

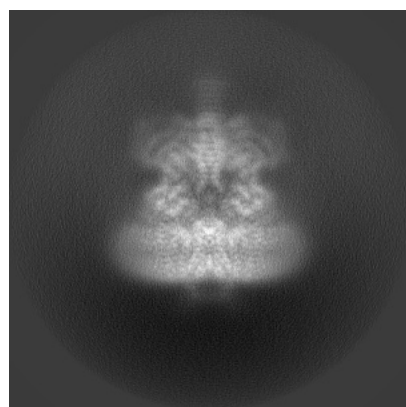


Y

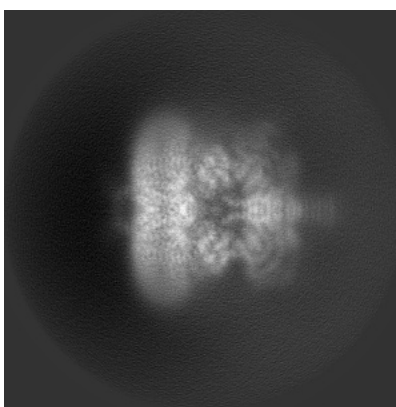


Z

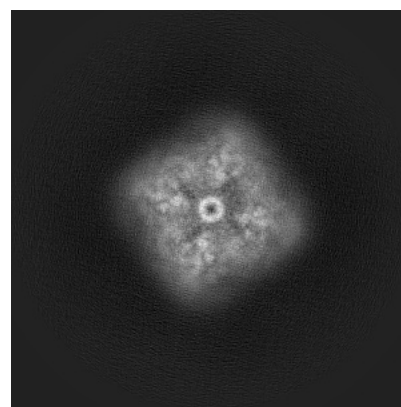
#### 6.1.2 Raw map



X



Y

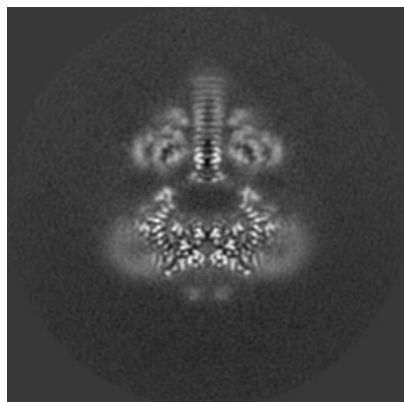


Z

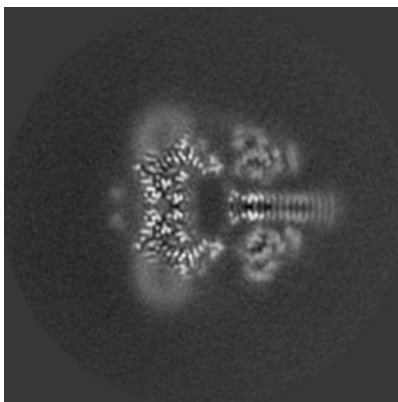
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

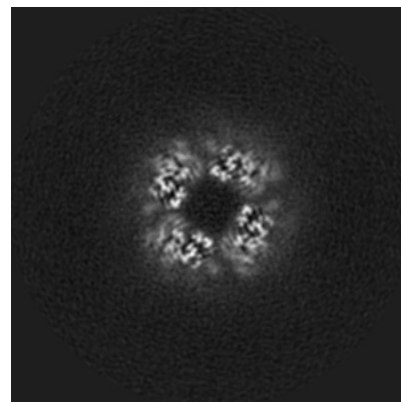
### 6.2.1 Primary map



X Index: 192

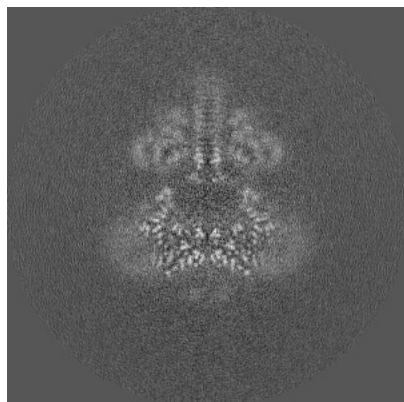


Y Index: 192

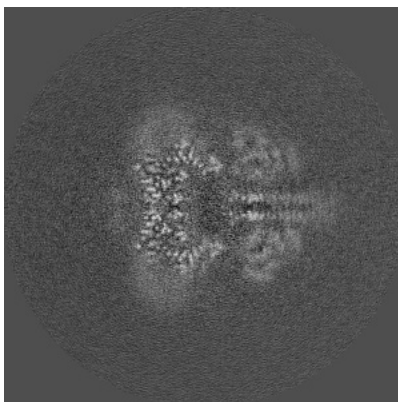


Z Index: 192

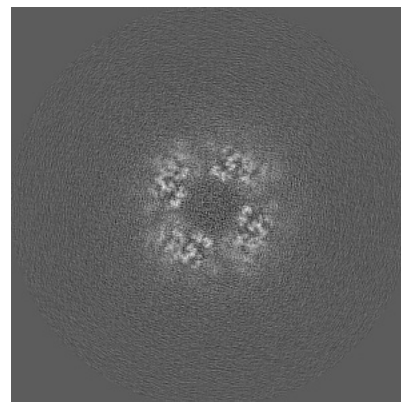
### 6.2.2 Raw map



X Index: 192



Y Index: 192

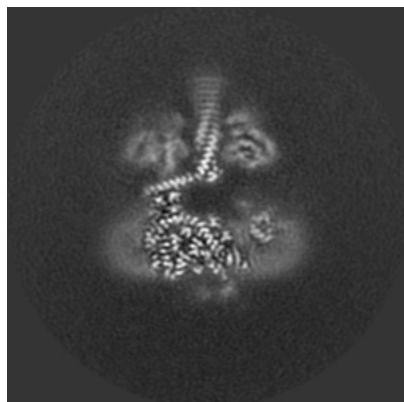


Z Index: 192

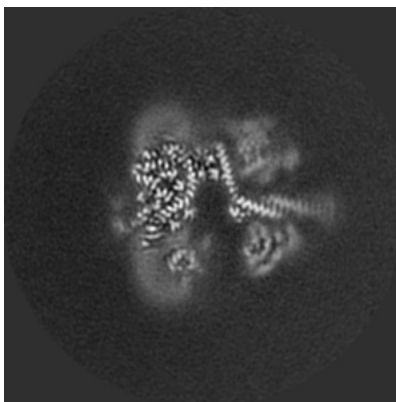
The images above show central slices of the map in three orthogonal directions.

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

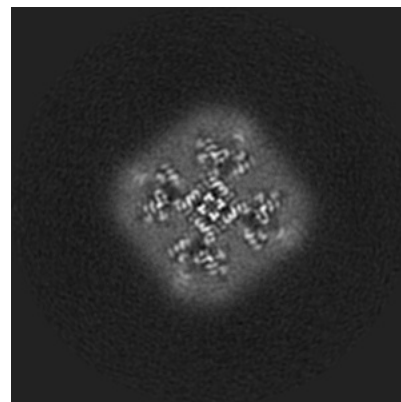
### 6.3.1 Primary map



X Index: 183

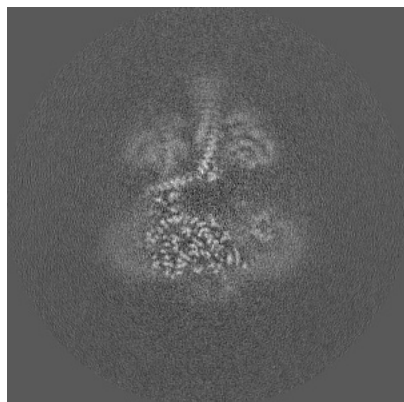


Y Index: 183

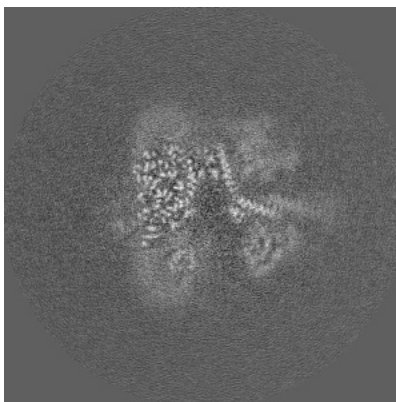


Z Index: 169

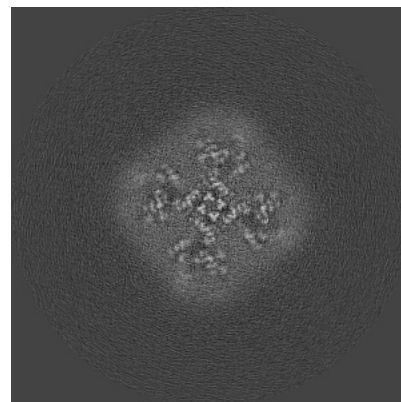
### 6.3.2 Raw map



X Index: 183



Y Index: 183



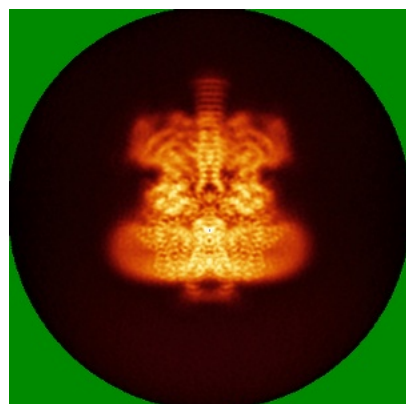
Z Index: 169

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

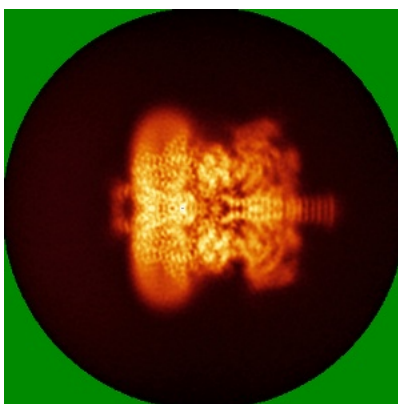


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

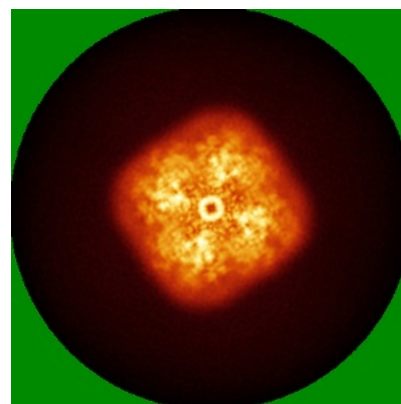
### 6.4.1 Primary map



X

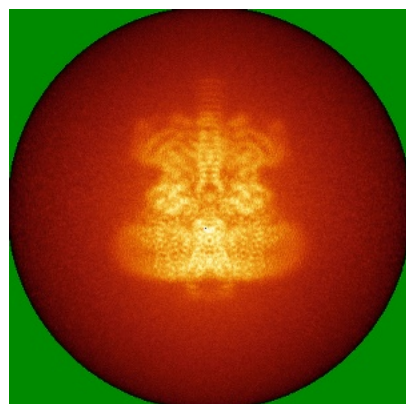


Y

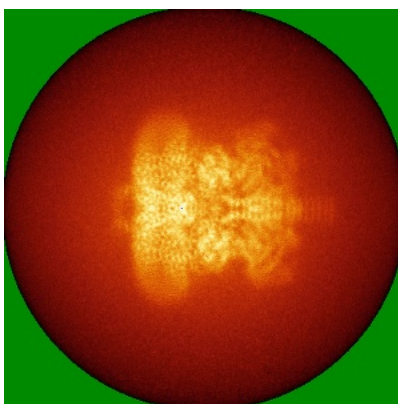


Z

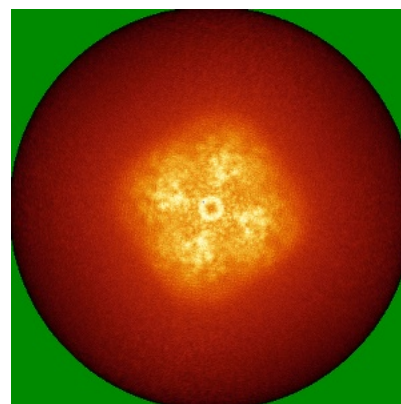
### 6.4.2 Raw map



X



Y

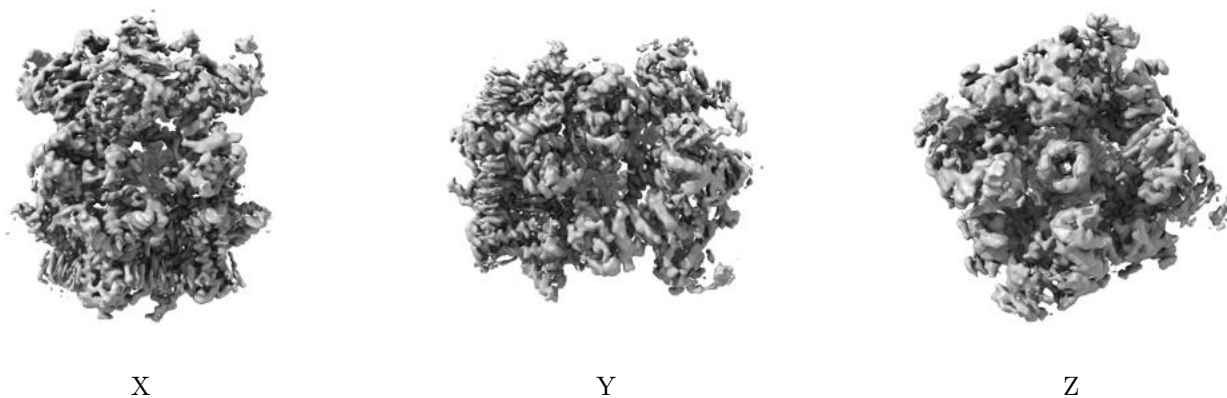


Z

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.

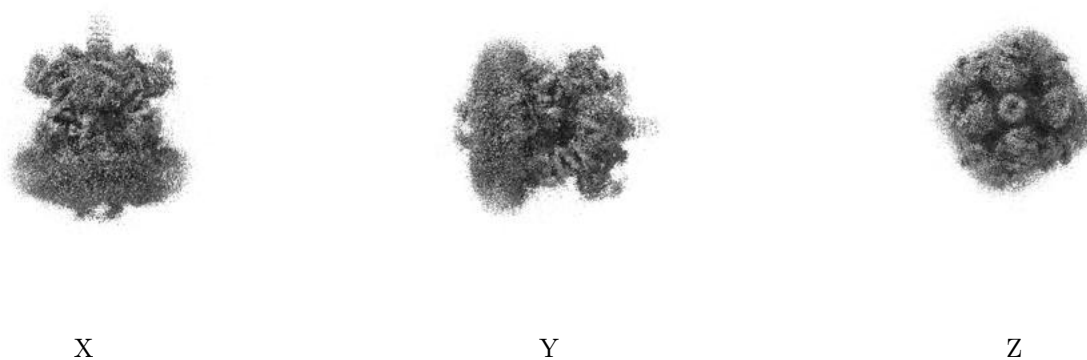
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0039. 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](#)

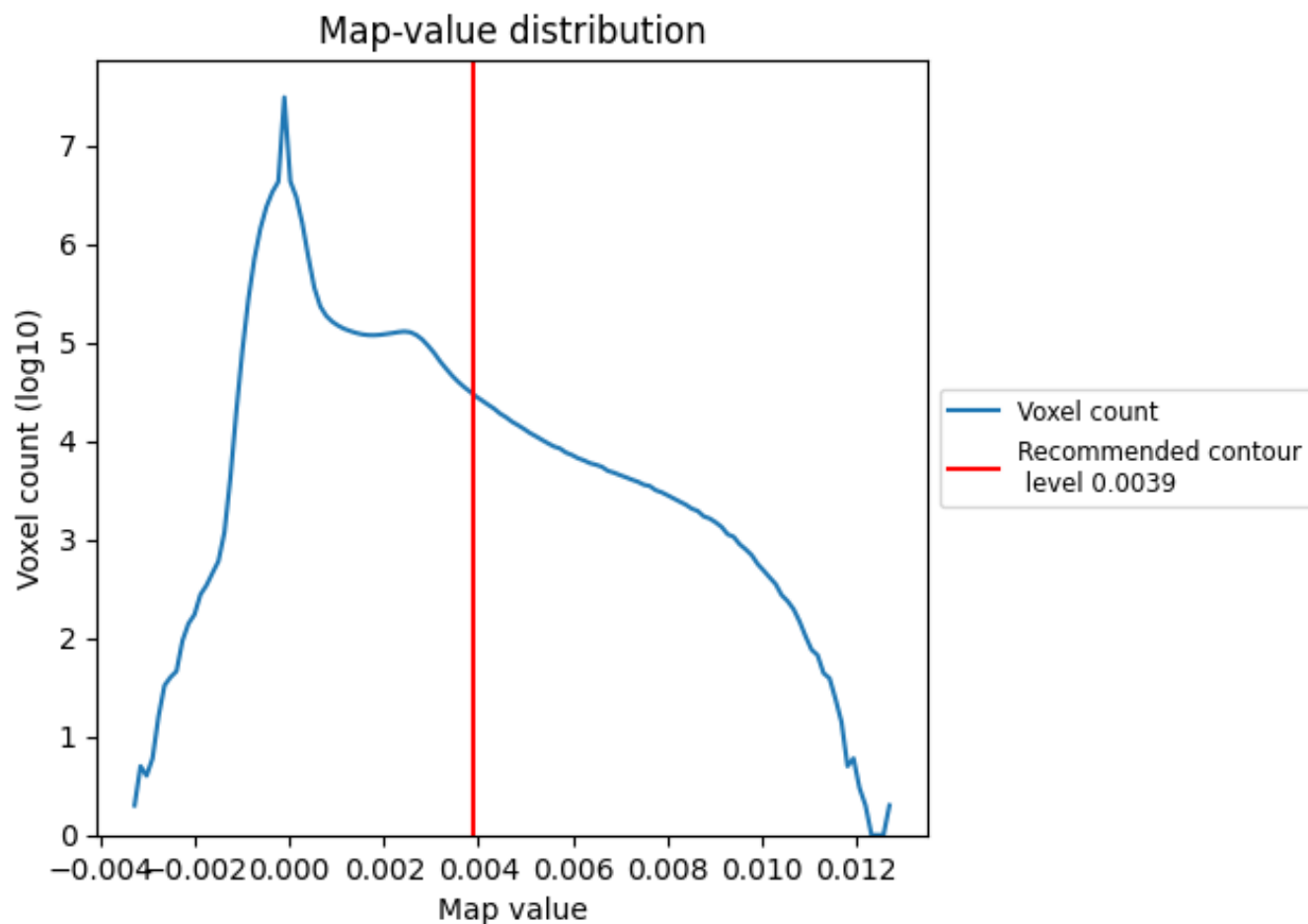
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

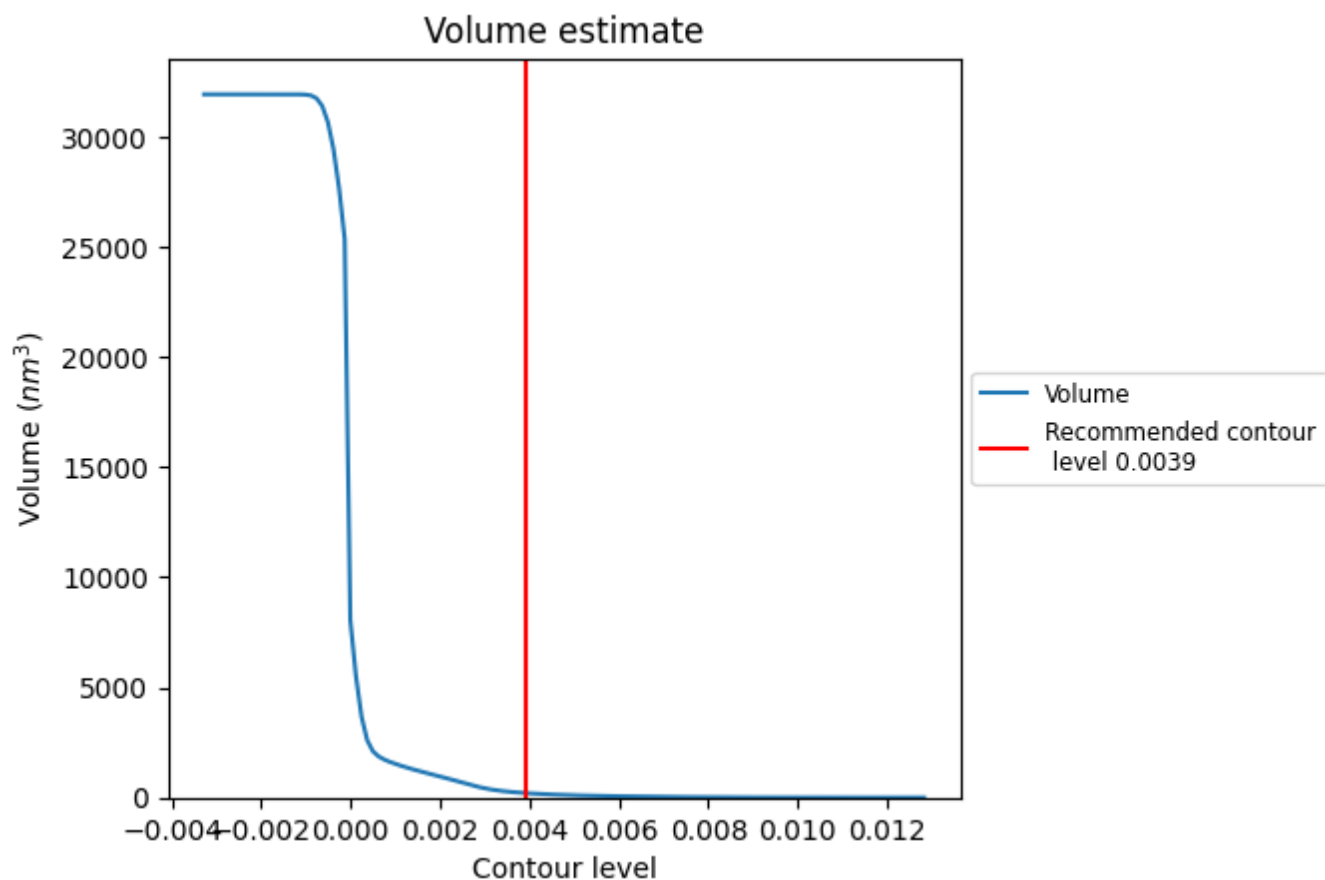
This section contains the results of statistical analysis of the map.

### 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.

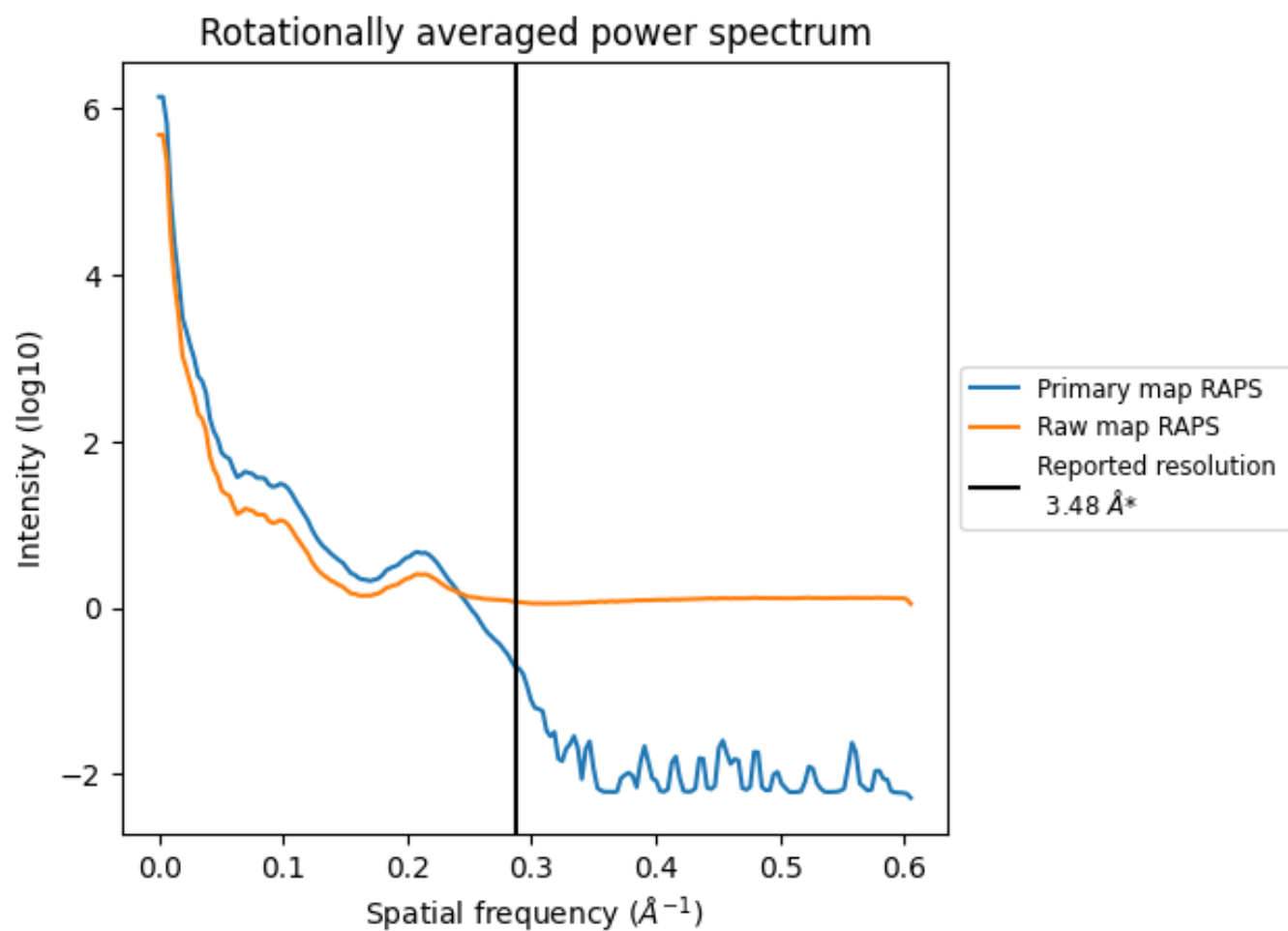
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 205 nm<sup>3</sup>; this corresponds to an approximate mass of 185 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](#)

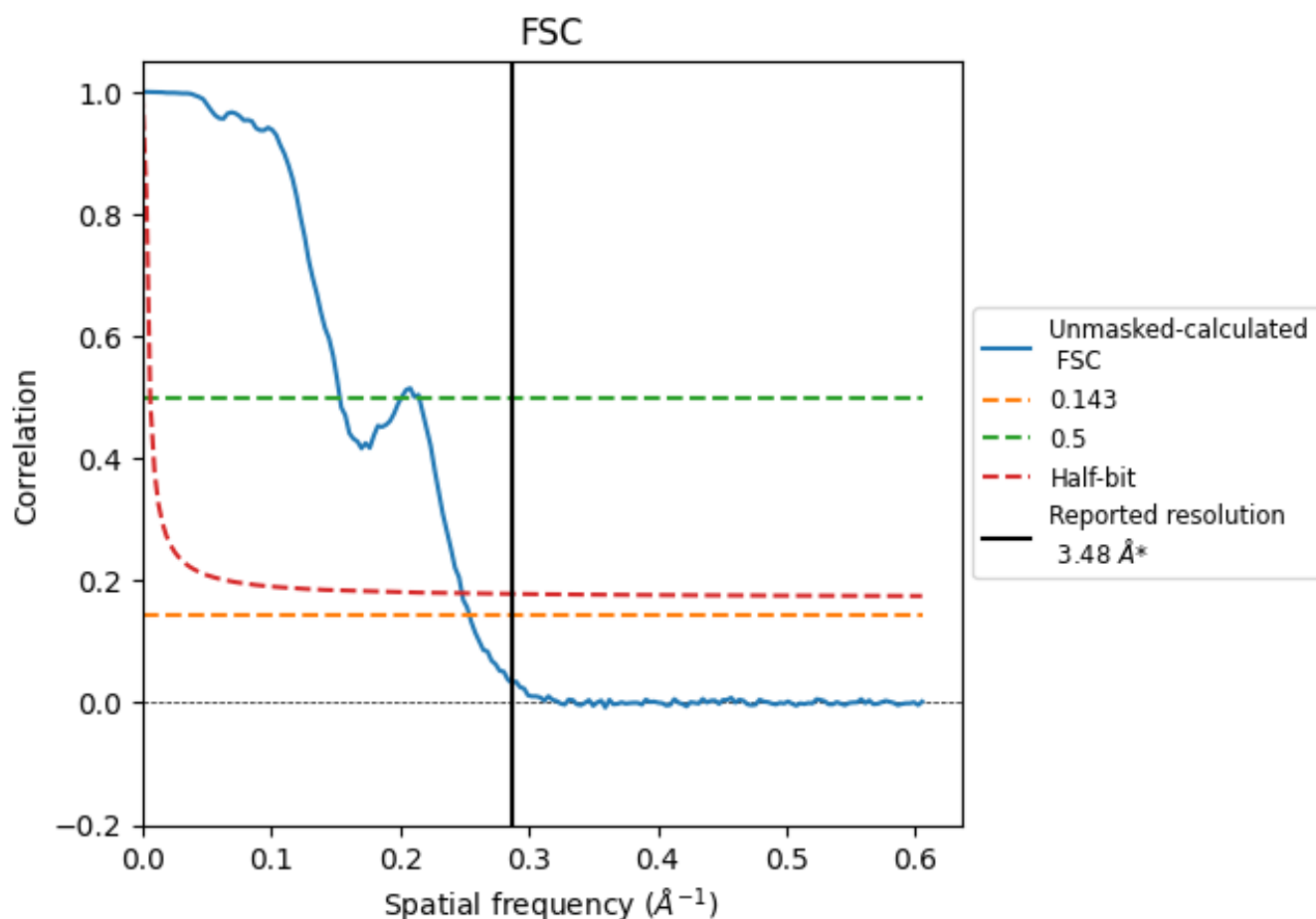


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.287  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

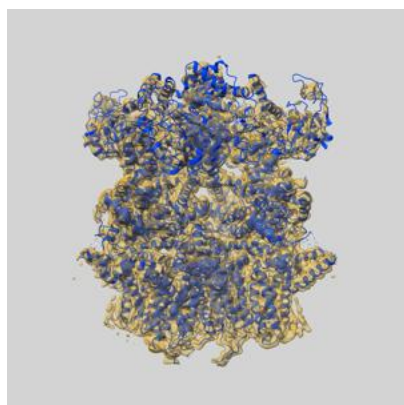
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.52	4.03

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.48 by more than 10 %

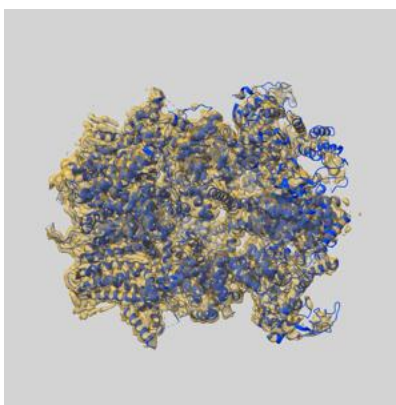
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70226 and PDB model 9O8G. Per-residue inclusion information can be found in section 3 on page 6.

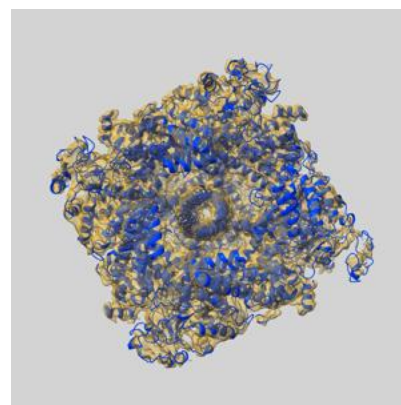
### 9.1 Map-model overlay [i](#)



X



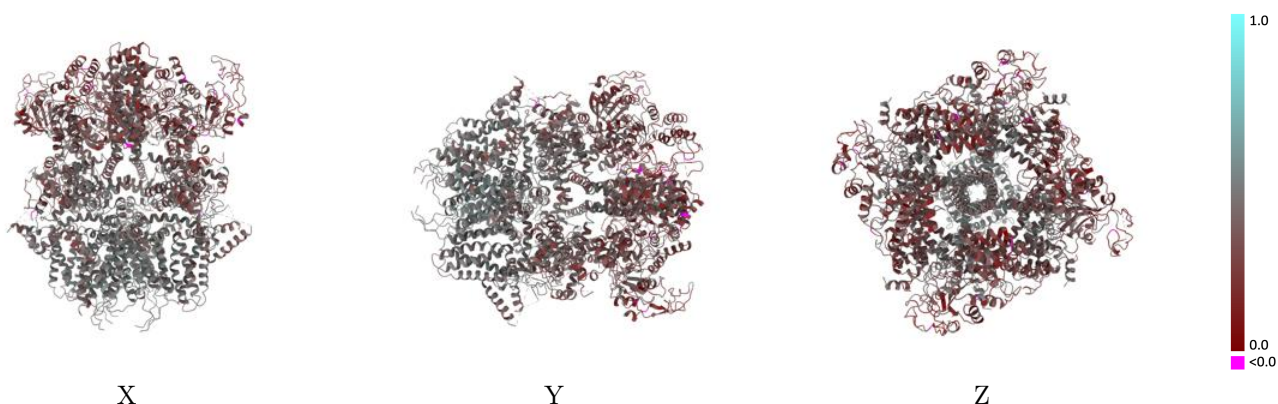
Y



Z

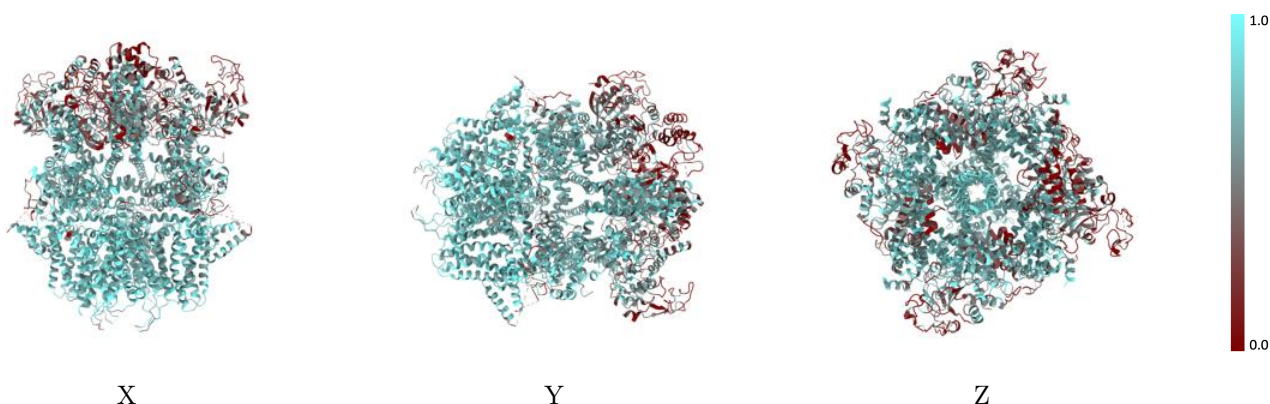
The images above show the 3D surface view of the map at the recommended contour level 0.0039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



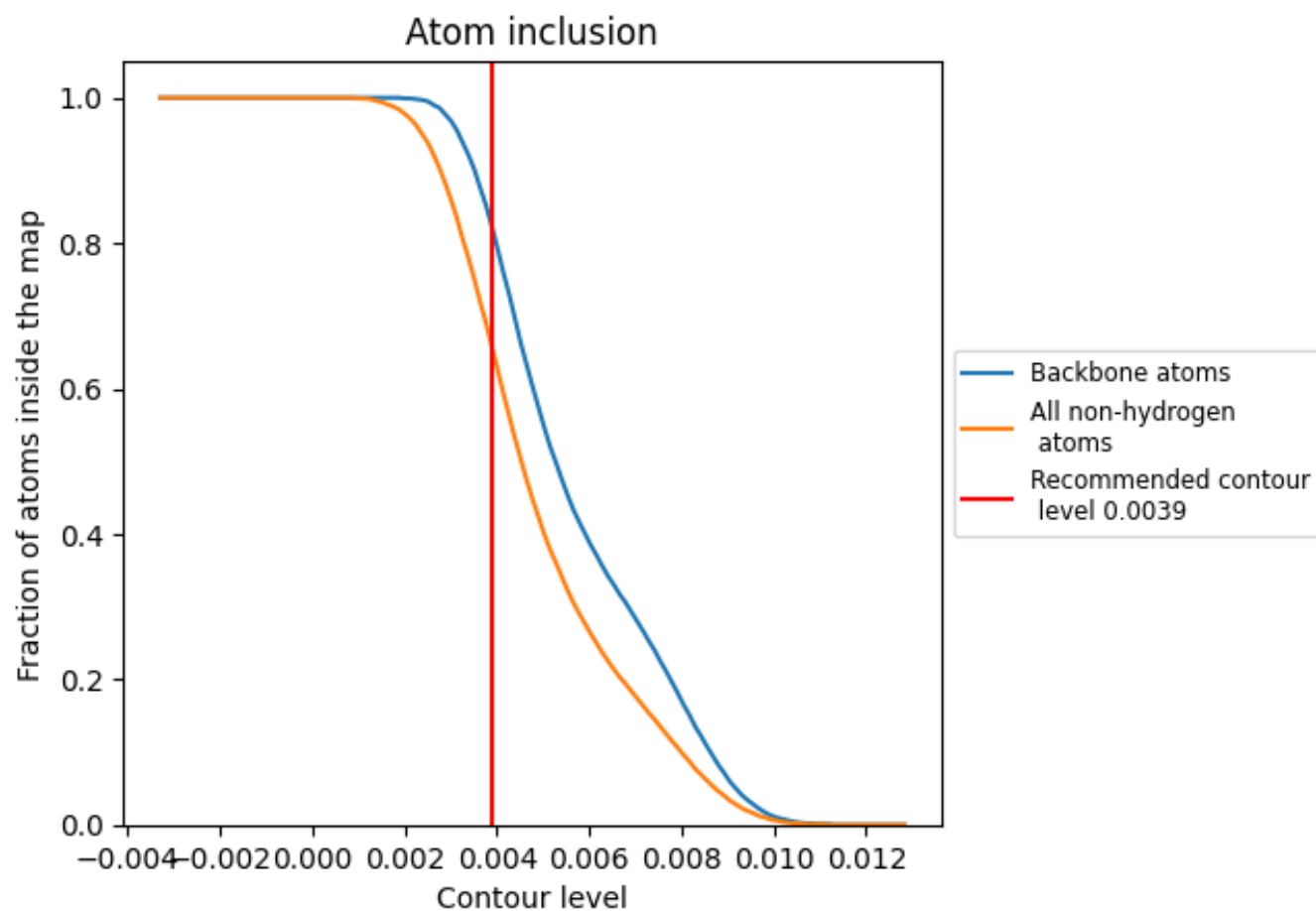
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0039).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.0039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6570	<div></div> 0.3860
A	<div></div> 0.6780	<div></div> 0.3870
B	<div></div> 0.6630	<div></div> 0.3810
C	<div></div> 0.5960	<div></div> 0.3860
D	<div></div> 0.6910	<div></div> 0.3900

