



Full wwPDB EM Validation Report ⓘ

Apr 25, 2026 – 11:25 PM EDT

PDB ID : 9PE1 / pdb_00009pe1
EMDB ID : EMD-71550
Title : Structure of beta-1,3-glucan synthase in complex with caspofungin, Rho1 and long glucan
Authors : Ren, Z.; Lee, S.Y.
Deposited on : 2025-07-01
Resolution : 3.09 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

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

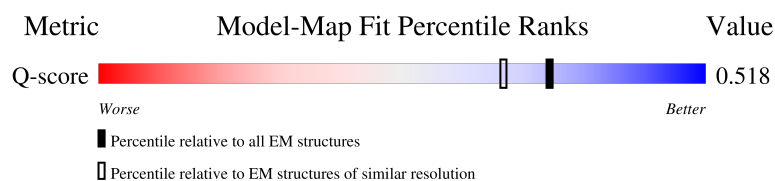
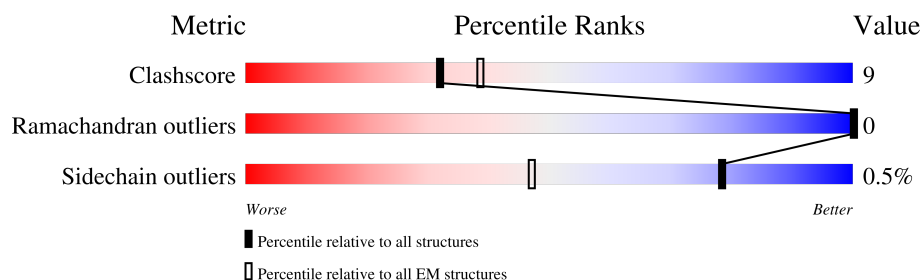
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 (2.59 - 3.59)

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	1931	
2	E	235	
3	G	197	
4	H	6	

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Mol	Chain	Length	Quality of chain
5	D	17	 76%24%
6	K	5	 60%40%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 32127 atoms, of which 15381 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 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1675	Total	C	H	N	O	S	0	0
			26592	8720	13201	2266	2330	75		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1877	LEU	-	expression tag	UNP P38631
A	1878	GLU	-	expression tag	UNP P38631
A	1879	VAL	-	expression tag	UNP P38631
A	1880	LEU	-	expression tag	UNP P38631
A	1881	PHE	-	expression tag	UNP P38631
A	1882	GLN	-	expression tag	UNP P38631
A	1883	GLY	-	expression tag	UNP P38631
A	1884	PRO	-	expression tag	UNP P38631
A	1885	ALA	-	expression tag	UNP P38631
A	1886	ALA	-	expression tag	UNP P38631
A	1887	ALA	-	expression tag	UNP P38631
A	1888	GLY	-	expression tag	UNP P38631
A	1889	SER	-	expression tag	UNP P38631
A	1890	ALA	-	expression tag	UNP P38631
A	1891	GLY	-	expression tag	UNP P38631
A	1892	SER	-	expression tag	UNP P38631
A	1893	ALA	-	expression tag	UNP P38631
A	1894	ALA	-	expression tag	UNP P38631
A	1895	GLY	-	expression tag	UNP P38631
A	1896	SER	-	expression tag	UNP P38631
A	1897	GLY	-	expression tag	UNP P38631
A	1898	GLU	-	expression tag	UNP P38631
A	1899	PHE	-	expression tag	UNP P38631
A	1900	ASP	-	expression tag	UNP P38631
A	1901	TYR	-	expression tag	UNP P38631
A	1902	LYS	-	expression tag	UNP P38631
A	1903	ASP	-	expression tag	UNP P38631
A	1904	HIS	-	expression tag	UNP P38631

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1905	ASP	-	expression tag	UNP P38631
A	1906	GLY	-	expression tag	UNP P38631
A	1907	ASP	-	expression tag	UNP P38631
A	1908	TYR	-	expression tag	UNP P38631
A	1909	LYS	-	expression tag	UNP P38631
A	1910	ASP	-	expression tag	UNP P38631
A	1911	HIS	-	expression tag	UNP P38631
A	1912	ASP	-	expression tag	UNP P38631
A	1913	ILE	-	expression tag	UNP P38631
A	1914	ASP	-	expression tag	UNP P38631
A	1915	TYR	-	expression tag	UNP P38631
A	1916	LYS	-	expression tag	UNP P38631
A	1917	ASP	-	expression tag	UNP P38631
A	1918	ASP	-	expression tag	UNP P38631
A	1919	ASP	-	expression tag	UNP P38631
A	1920	ASP	-	expression tag	UNP P38631
A	1921	LYS	-	expression tag	UNP P38631
A	1922	HIS	-	expression tag	UNP P38631
A	1923	HIS	-	expression tag	UNP P38631
A	1924	HIS	-	expression tag	UNP P38631
A	1925	HIS	-	expression tag	UNP P38631
A	1926	HIS	-	expression tag	UNP P38631
A	1927	HIS	-	expression tag	UNP P38631
A	1928	HIS	-	expression tag	UNP P38631
A	1929	HIS	-	expression tag	UNP P38631
A	1930	HIS	-	expression tag	UNP P38631
A	1931	HIS	-	expression tag	UNP P38631

- Molecule 2 is a protein called GTP-binding protein RHO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	179	Total	C	H	N	O	S	0	0
			2570	840	1250	227	249	4		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP P06780
E	-24	GLY	-	expression tag	UNP P06780
E	-23	SER	-	expression tag	UNP P06780
E	-22	SER	-	expression tag	UNP P06780
E	-21	HIS	-	expression tag	UNP P06780

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	HIS	-	expression tag	UNP P06780
E	-19	HIS	-	expression tag	UNP P06780
E	-18	HIS	-	expression tag	UNP P06780
E	-17	HIS	-	expression tag	UNP P06780
E	-16	HIS	-	expression tag	UNP P06780
E	-15	SER	-	expression tag	UNP P06780
E	-14	SER	-	expression tag	UNP P06780
E	-13	GLY	-	expression tag	UNP P06780
E	-12	LEU	-	expression tag	UNP P06780
E	-11	VAL	-	expression tag	UNP P06780
E	-10	PRO	-	expression tag	UNP P06780
E	-9	ARG	-	expression tag	UNP P06780
E	-8	GLY	-	expression tag	UNP P06780
E	-7	SER	-	expression tag	UNP P06780
E	-6	HIS	-	expression tag	UNP P06780
E	-5	MET	-	expression tag	UNP P06780
E	-4	GLU	-	expression tag	UNP P06780
E	-3	ASN	-	expression tag	UNP P06780
E	-2	LEU	-	expression tag	UNP P06780
E	-1	TYR	-	expression tag	UNP P06780
E	0	PHE	-	expression tag	UNP P06780
E	1	GLN	-	expression tag	UNP P06780

- | Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 3 | G | 72 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1086 | 358 | 521 | 97 | 109 | 1 | | |

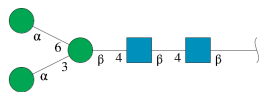
- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|---|
| 4 | H | 6 | Total
120 | C
36 | H
60 | N
10 | O
14 | 0 | 0 |

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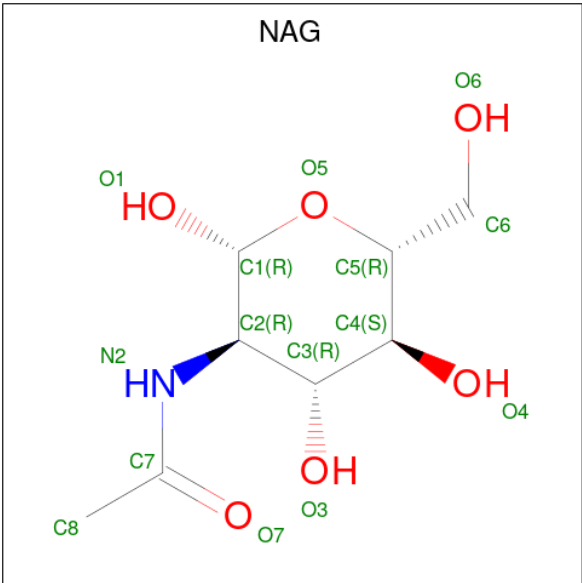
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	17	Total	C	H	O	0	0
			344	102	156	86		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



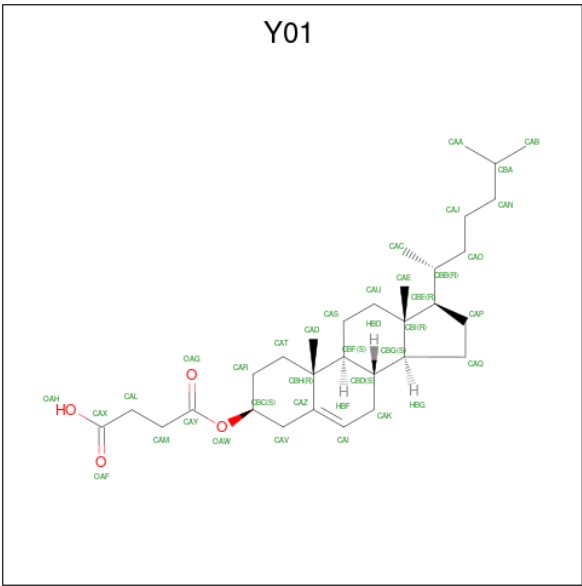
Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



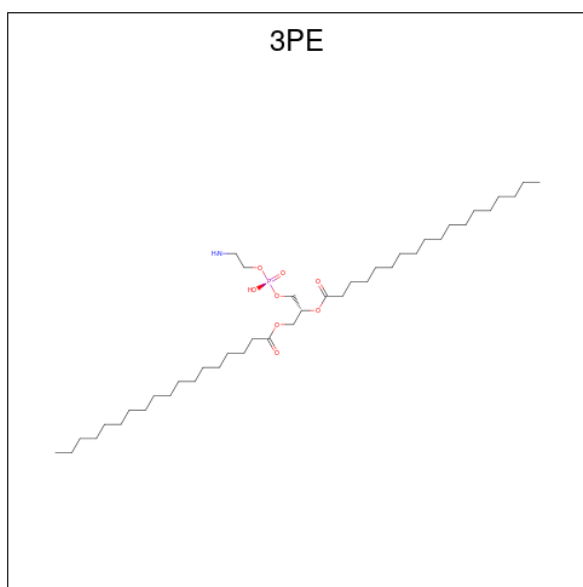
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31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

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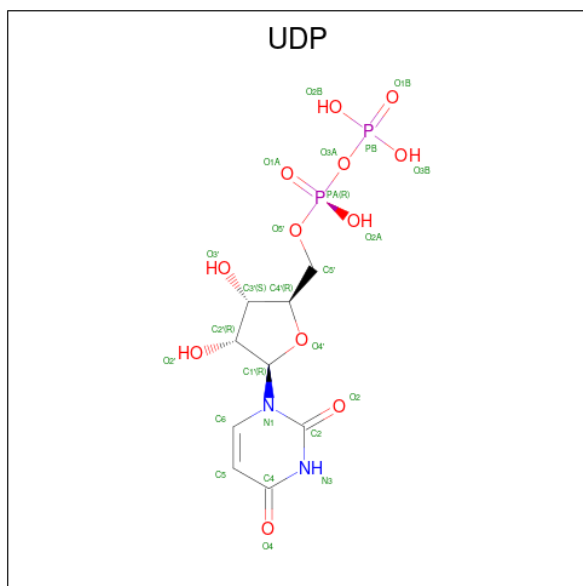
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31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

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



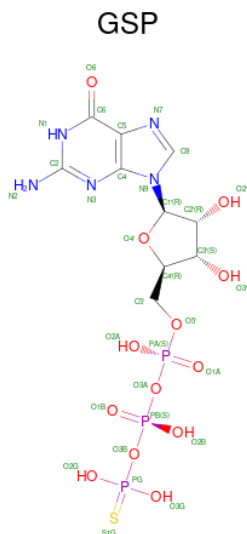
Mol	Chain	Residues	Atoms					AltConf	
9	A	1	Total	C	H	N	O	P	0
			123	39	74	1	8	1	

- Molecule 10 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



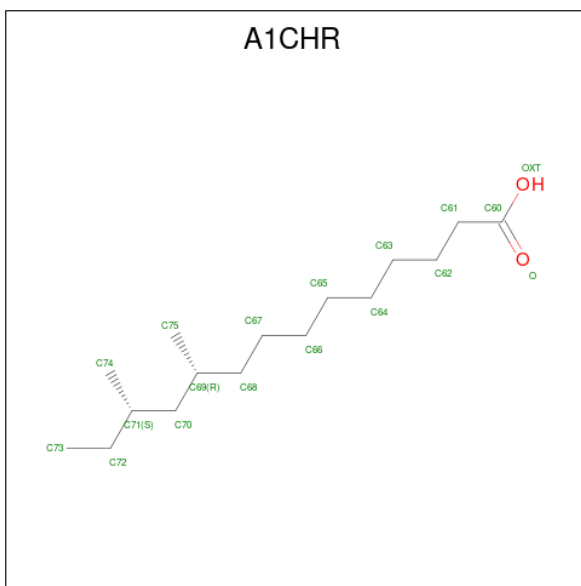
Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

- Molecule 11 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms							AltConf
11	E	1	Total	C	H	N	O	P	S	0
			44	10	12	5	13	3	1	

- Molecule 12 is (10R,12S)-10,12-dimethyltetradecanoic acid (CCD ID: A1CHR) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	H	1	Total	C	H	O	0
			48	16	31	1	

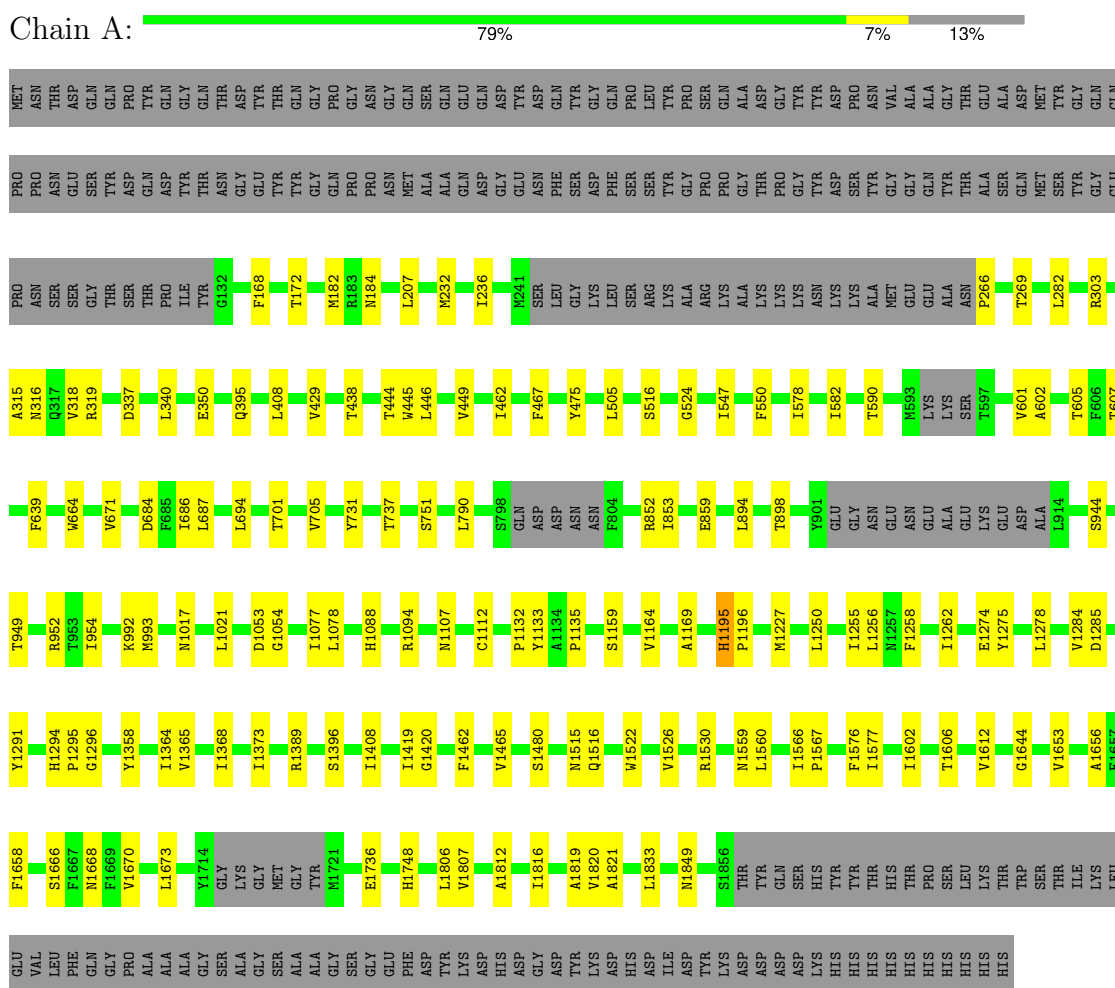
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	9	Total	O	0
			9	9	

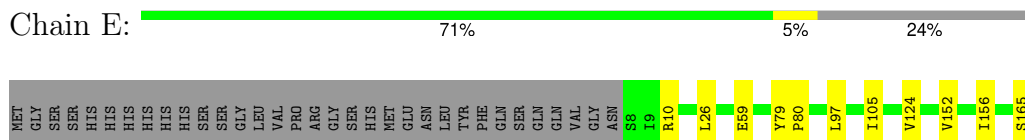
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 1,3-beta-glucan synthase component FKS1



- Molecule 2: GTP-binding protein RHO1





WORLD WIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.425	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.0792	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 3PE, Y01, HY3, A1CHU, A1CHT, BGC, NAG, A1CHS, A1CHR, UDP, MAN, BMA, HYP, GSP

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	0.15	0/13750	0.30	0/18670
2	E	0.17	0/1345	0.32	0/1834
3	G	0.10	0/581	0.27	0/794
4	H	0.41	0/6	1.54	0/7
All	All	0.15	0/15682	0.30	0/21305

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
4	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	2	A1CHS	Peptide

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	13391	13201	13201	112	0
2	E	1320	1250	1250	6	0
3	G	565	521	521	5	0
4	H	60	60	16	2	0
5	D	188	156	155	3	0
6	K	61	52	52	0	0
7	A	14	13	13	0	0
8	A	980	0	1372	198	0
8	H	35	0	49	7	0
9	A	49	74	75	2	0
10	A	25	11	10	0	0
11	E	32	12	12	0	0
12	H	17	31	0	0	0
13	A	9	0	0	0	0
All	All	16746	15381	16726	286	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 9.

All (286) 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)
8:A:2002:Y01:HAD3	8:A:2013:Y01:HAI	1.43	0.96
8:A:2022:Y01:HAS1	8:H:102:Y01:HAK1	1.48	0.95
8:A:2014:Y01:HAL2	8:A:2016:Y01:HAL1	1.46	0.95
8:A:2010:Y01:HAB3	8:A:2015:Y01:HAA3	1.47	0.95
8:A:2002:Y01:HAU1	8:A:2004:Y01:HAB3	1.48	0.93
8:A:2014:Y01:HAR1	8:A:2016:Y01:HAR1	1.53	0.89
8:A:2023:Y01:HAC1	8:A:2023:Y01:HAE2	1.63	0.81
8:A:2003:Y01:HAE2	8:A:2003:Y01:HAC1	1.66	0.77
8:A:2022:Y01:HAK1	8:A:2023:Y01:HAK1	1.65	0.76
8:A:2022:Y01:HAQ2	8:A:2023:Y01:HAQ1	1.68	0.76
8:A:2012:Y01:HBC	8:A:2012:Y01:HAL1	1.69	0.75
1:A:516:SER:HB2	8:A:2007:Y01:HAV2	1.73	0.70
1:A:1656:ALA:HA	8:A:2018:Y01:HAC3	1.75	0.69
8:A:2017:Y01:HAP1	8:A:2017:Y01:HAJ1	1.72	0.69
8:A:2011:Y01:OAG	8:A:2012:Y01:HAD1	1.92	0.68
8:A:2005:Y01:HAA1	8:A:2005:Y01:HAP2	1.74	0.68
1:A:184:ASN:OD1	1:A:1094:ARG:NH2	2.27	0.67
1:A:449:VAL:HG22	8:A:2013:Y01:HAJ1	1.77	0.67
8:A:2005:Y01:HAJ2	8:A:2005:Y01:HAP1	1.77	0.66
1:A:444:THR:HG22	1:A:446:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:ALA:HB2	1:A:1255:ILE:HD11	1.76	0.66
1:A:462:ILE:HD11	8:A:2003:Y01:HAD3	1.78	0.66
8:A:2007:Y01:HAE2	8:A:2007:Y01:HAC1	1.78	0.66
8:A:2028:Y01:HAU2	8:A:2028:Y01:HAC1	1.77	0.65
8:A:2013:Y01:HAU2	8:A:2013:Y01:HAC1	1.79	0.65
8:A:2023:Y01:HAJ1	8:A:2023:Y01:CAP	2.25	0.65
1:A:1606:THR:HG21	8:A:2016:Y01:HAB3	1.79	0.65
8:A:2005:Y01:HAA1	8:A:2005:Y01:CAP	2.27	0.65
8:A:2017:Y01:HAR1	8:A:2017:Y01:CAX	2.27	0.64
1:A:1227:MET:HE2	1:A:1274:GLU:HB3	1.80	0.64
1:A:1169:ALA:HB2	1:A:1255:ILE:CD1	2.28	0.63
8:A:2003:Y01:HAL2	8:A:2024:Y01:HAK2	1.80	0.63
8:A:2011:Y01:HAU2	8:A:2011:Y01:HAC1	1.80	0.63
8:A:2030:Y01:HAE2	8:A:2030:Y01:HAC1	1.81	0.63
8:A:2003:Y01:CAL	8:A:2024:Y01:HAK2	2.29	0.62
1:A:1227:MET:HE1	1:A:1275:TYR:CD1	2.35	0.61
8:A:2014:Y01:HAC2	8:A:2016:Y01:HAC2	1.82	0.61
1:A:1656:ALA:CA	8:A:2018:Y01:HAC3	2.30	0.61
8:A:2023:Y01:HAJ1	8:A:2023:Y01:HAP2	1.81	0.61
8:A:2003:Y01:HAM2	8:A:2024:Y01:HBG	1.82	0.61
1:A:1530:ARG:NH2	1:A:1736:GLU:OE2	2.33	0.61
8:A:2010:Y01:HAA1	8:A:2013:Y01:HAA2	1.82	0.61
8:A:2022:Y01:HAE2	8:A:2022:Y01:HAC1	1.83	0.61
8:A:2005:Y01:HAD3	8:A:2005:Y01:HAE1	1.83	0.60
1:A:894:LEU:O	1:A:898:THR:HG23	2.01	0.60
8:A:2010:Y01:HAC1	8:A:2010:Y01:HAU2	1.83	0.59
1:A:446:LEU:HD13	8:A:2007:Y01:HAS1	1.84	0.59
1:A:1227:MET:HE3	1:A:1278:LEU:HD12	1.84	0.59
8:A:2009:Y01:HAP1	8:A:2009:Y01:HAJ1	1.83	0.59
8:A:2009:Y01:HAD3	8:A:2009:Y01:HAE1	1.84	0.59
1:A:315:ALA:HB1	1:A:318:VAL:HB	1.84	0.58
1:A:1559:ASN:ND2	8:A:2010:Y01:HAL1	2.19	0.58
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAE2	1.84	0.58
8:A:2030:Y01:HAJ1	8:A:2030:Y01:HAP1	1.86	0.58
8:A:2008:Y01:HAJ1	8:A:2008:Y01:HAP1	1.85	0.58
8:A:2017:Y01:HAC1	8:A:2017:Y01:HAU2	1.86	0.58
8:A:2016:Y01:HAJ2	8:A:2016:Y01:HAP1	1.86	0.57
8:A:2020:Y01:HBG	8:A:2028:Y01:HAD1	1.85	0.57
1:A:1368:ILE:O	1:A:1368:ILE:HG22	2.04	0.57
8:A:2010:Y01:HAA1	8:A:2013:Y01:CAA	2.35	0.57
8:H:102:Y01:HAC1	8:H:102:Y01:HAU2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2029:Y01:HAE1	8:A:2029:Y01:HAD3	1.85	0.57
3:G:127:GLU:OE1	3:G:136:ARG:NH1	2.38	0.57
1:A:671:VAL:HG12	1:A:671:VAL:O	2.04	0.56
1:A:475:TYR:HB3	8:A:2012:Y01:HAK1	1.86	0.56
2:E:124:VAL:N	2:E:165:SER:OG	2.38	0.56
1:A:1294:HIS:HB2	1:A:1295:PRO:HD3	1.87	0.56
8:A:2008:Y01:CAK	8:A:2018:Y01:HAM2	2.35	0.56
8:A:2020:Y01:HAC1	8:A:2020:Y01:HAU2	1.86	0.56
8:A:2021:Y01:HAD3	8:A:2021:Y01:HAE1	1.87	0.56
8:A:2022:Y01:CAS	8:H:102:Y01:HAK1	2.30	0.56
8:A:2012:Y01:HAC1	8:A:2012:Y01:HAU2	1.87	0.56
8:A:2014:Y01:HAI	8:A:2029:Y01:CAD	2.37	0.55
8:A:2016:Y01:HAC1	8:A:2016:Y01:HAU2	1.88	0.55
1:A:1816:ILE:HG12	8:A:2020:Y01:HAS2	1.89	0.55
1:A:315:ALA:O	1:A:319:ARG:NH1	2.39	0.55
1:A:664:TRP:HB2	8:A:2014:Y01:HAR2	1.87	0.55
1:A:1577:ILE:HD12	8:A:2005:Y01:HAA2	1.88	0.55
8:A:2008:Y01:HAE1	8:A:2008:Y01:HAD3	1.87	0.55
1:A:1820:VAL:HG12	8:A:2019:Y01:HAK1	1.87	0.55
1:A:1821:ALA:HB2	8:A:2019:Y01:HAK2	1.89	0.55
8:A:2012:Y01:HAS1	8:A:2015:Y01:HAK2	1.88	0.55
1:A:350:GLU:OE1	3:G:101:ARG:NH1	2.39	0.55
1:A:505:LEU:HD22	8:A:2015:Y01:HAA1	1.88	0.55
1:A:269:THR:HG21	1:A:1135:PRO:HB3	1.90	0.54
8:A:2014:Y01:HAL2	8:A:2016:Y01:CAL	2.31	0.54
1:A:1053:ASP:OD1	1:A:1054:GLY:N	2.41	0.54
1:A:1480:SER:OG	8:A:2021:Y01:HAA2	2.08	0.54
1:A:172:THR:HG21	1:A:182:MET:HB2	1.89	0.53
1:A:701:THR:O	1:A:705:VAL:HG23	2.08	0.53
8:A:2009:Y01:HAK1	8:A:2019:Y01:HBFB	1.90	0.53
1:A:578:ILE:HG12	8:A:2003:Y01:HAU2	1.91	0.53
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAU2	1.91	0.53
8:A:2020:Y01:HBG	8:A:2028:Y01:CAD	2.39	0.53
8:A:2027:Y01:CAJ	8:A:2027:Y01:HAP1	2.31	0.52
1:A:664:TRP:CB	8:A:2014:Y01:HAR2	2.39	0.52
8:A:2008:Y01:HAC1	8:A:2008:Y01:HAU2	1.92	0.52
1:A:303:ARG:NH2	1:A:337:ASP:OD1	2.43	0.52
8:A:2012:Y01:HBC	8:A:2012:Y01:CAL	2.32	0.52
8:A:2009:Y01:HAE1	8:A:2009:Y01:CAD	2.40	0.51
8:A:2024:Y01:CAJ	8:A:2024:Y01:HAP1	2.39	0.51
8:A:2005:Y01:HAE2	8:A:2005:Y01:HAC1	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2022:Y01:HAC1	8:A:2022:Y01:HAU2	1.92	0.51
1:A:1576:PHE:CD1	8:A:2014:Y01:HAC3	2.45	0.51
1:A:1656:ALA:CB	8:A:2018:Y01:HAC3	2.40	0.51
4:H:3:THR:CG2	8:H:102:Y01:HAL1	2.40	0.51
1:A:751:SER:HB3	1:A:790:LEU:HD21	1.93	0.51
1:A:1666:SER:O	1:A:1668:ASN:N	2.43	0.51
1:A:1819:ALA:CB	8:A:2020:Y01:HAR1	2.41	0.51
2:E:10:ARG:NE	2:E:59:GLU:OE2	2.43	0.51
1:A:266:PRO:N	1:A:269:THR:HG23	2.26	0.51
8:A:2021:Y01:OAG	8:A:2021:Y01:HAR2	2.11	0.51
1:A:1812:ALA:CB	8:A:2020:Y01:HAC3	2.41	0.50
1:A:505:LEU:CD2	8:A:2015:Y01:HAA1	2.40	0.50
8:A:2029:Y01:HAE1	8:A:2029:Y01:CAD	2.41	0.50
1:A:1419:ILE:HG22	1:A:1560:LEU:HD21	1.94	0.50
8:A:2008:Y01:HAV2	8:A:2008:Y01:HAM1	1.94	0.50
1:A:1612:VAL:HG11	1:A:1653:VAL:HG21	1.93	0.49
1:A:1748:HIS:ND1	1:A:1807:VAL:HG11	2.28	0.49
1:A:731:TYR:CZ	1:A:737:THR:HG21	2.48	0.49
8:A:2012:Y01:HAR2	8:A:2015:Y01:HAI	1.94	0.49
8:A:2020:Y01:HAC1	8:A:2020:Y01:HAE2	1.95	0.49
1:A:236:ILE:HD13	1:A:605:THR:HG22	1.93	0.49
8:A:2007:Y01:HAC1	8:A:2007:Y01:HAU2	1.94	0.49
8:A:2018:Y01:OAG	8:A:2018:Y01:HAV1	2.12	0.49
1:A:505:LEU:HD21	8:A:2007:Y01:HAA2	1.95	0.49
1:A:1258:PHE:CZ	1:A:1262:ILE:HD11	2.48	0.49
1:A:1164:VAL:HG21	1:A:1396:SER:HB3	1.95	0.48
1:A:1833:LEU:HD22	8:A:2008:Y01:HAM2	1.94	0.48
8:A:2008:Y01:HAK1	8:A:2018:Y01:OAG	2.13	0.48
1:A:446:LEU:CD1	8:A:2007:Y01:HAS1	2.43	0.48
1:A:467:PHE:HB3	8:A:2012:Y01:HAA1	1.95	0.48
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAU2	1.95	0.48
8:A:2029:Y01:HAC1	8:A:2029:Y01:HAU2	1.96	0.48
8:A:2023:Y01:CAC	8:A:2023:Y01:HAU2	2.43	0.48
8:A:2022:Y01:HAJ1	8:A:2022:Y01:HAP1	1.96	0.48
1:A:408:LEU:HD23	1:A:429:VAL:HG22	1.96	0.48
1:A:1806:LEU:HD13	8:A:2027:Y01:HAC3	1.96	0.48
3:G:138:ASP:OD1	3:G:138:ASP:C	2.56	0.48
8:A:2003:Y01:HAR1	8:A:2024:Y01:CAP	2.43	0.47
8:A:2010:Y01:CAB	8:A:2015:Y01:HAA3	2.32	0.47
8:A:2018:Y01:HAP1	8:A:2018:Y01:HAO2	1.52	0.47
8:A:2011:Y01:OAG	8:A:2011:Y01:HAR1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ILE:CG2	1:A:1021:LEU:HD11	2.44	0.47
1:A:1017:ASN:O	1:A:1021:LEU:HD13	2.14	0.47
8:A:2005:Y01:HAD1	8:A:2014:Y01:HAI	1.96	0.47
8:A:2014:Y01:HAB1	8:A:2014:Y01:HAO1	1.96	0.47
8:A:2026:Y01:HAE2	8:A:2026:Y01:HBB	1.69	0.47
2:E:105:ILE:HD12	2:E:156:ILE:HB	1.96	0.47
1:A:944:SER:HB3	1:A:949:THR:HG21	1.97	0.47
1:A:686:ILE:HD11	8:A:2002:Y01:HAQ2	1.96	0.47
1:A:1373:ILE:HD11	1:A:1389:ARG:HE	1.79	0.46
1:A:1812:ALA:HB1	8:A:2020:Y01:HAC3	1.97	0.46
5:D:9:BGC:O4	5:D:10:BGC:O5	2.32	0.46
1:A:395:GLN:HB2	1:A:438:THR:HG21	1.96	0.46
1:A:1656:ALA:HB1	8:A:2018:Y01:HAC3	1.96	0.46
8:A:2025:Y01:HAP1	8:A:2025:Y01:HAO2	1.31	0.46
8:A:2003:Y01:HAK2	8:A:2023:Y01:HAC2	1.96	0.46
8:A:2009:Y01:HAS2	8:A:2009:Y01:HAT2	1.49	0.46
8:A:2022:Y01:CAK	8:A:2023:Y01:HAK1	2.40	0.46
1:A:731:TYR:CE1	1:A:737:THR:HG21	2.50	0.46
1:A:1291:TYR:O	1:A:1296:GLY:N	2.49	0.46
8:A:2017:Y01:HAC1	8:A:2017:Y01:HAE2	1.98	0.46
8:A:2019:Y01:HAC2	8:A:2019:Y01:HAJ2	1.66	0.46
8:A:2003:Y01:HAE2	8:A:2003:Y01:CAC	2.42	0.45
8:A:2008:Y01:HAC1	8:A:2008:Y01:HAE2	1.99	0.45
8:A:2025:Y01:CAZ	8:A:2027:Y01:HAR1	2.46	0.45
1:A:1419:ILE:HG13	1:A:1420:GLY:N	2.31	0.45
8:A:2018:Y01:HAE2	8:A:2018:Y01:HBB	1.72	0.45
1:A:1077:ILE:O	1:A:1078:LEU:C	2.59	0.45
1:A:1256:LEU:HD22	1:A:1408:ILE:HD12	1.98	0.45
8:A:2019:Y01:OAG	8:A:2019:Y01:HAV2	2.16	0.45
5:D:15:BGC:O4	5:D:16:BGC:O5	2.31	0.45
8:A:2012:Y01:HAD2	8:A:2012:Y01:HAS2	1.85	0.45
8:A:2025:Y01:HAO1	8:A:2025:Y01:HBA	1.38	0.45
8:A:2016:Y01:HAC1	8:A:2016:Y01:HAE2	1.98	0.45
8:A:2010:Y01:HAD3	8:A:2010:Y01:HBD	1.82	0.45
1:A:547:ILE:HG12	8:A:2015:Y01:HAS2	1.99	0.44
1:A:1515:ASN:OD1	1:A:1516:GLN:N	2.49	0.44
8:A:2018:Y01:HAD3	8:A:2018:Y01:HBD	1.77	0.44
8:A:2027:Y01:HAP1	8:A:2027:Y01:HAJ2	1.99	0.44
8:A:2022:Y01:HAS2	8:A:2022:Y01:HAD2	1.69	0.44
1:A:445:TRP:HB2	8:A:2010:Y01:HAR1	1.99	0.44
1:A:1566:ILE:HB	1:A:1567:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:PHE:CE2	3:G:126:LEU:HD11	2.52	0.44
8:A:2013:Y01:HAC1	8:A:2013:Y01:CAU	2.46	0.44
8:A:2002:Y01:HAO1	8:A:2010:Y01:HAO1	1.99	0.44
8:A:2010:Y01:CAC	8:A:2013:Y01:HAP2	2.48	0.44
8:A:2029:Y01:HAT2	8:A:2029:Y01:HAS2	1.49	0.44
2:E:79:TYR:O	2:E:80:PRO:C	2.61	0.44
1:A:168:PHE:O	1:A:172:THR:HG23	2.18	0.44
1:A:207:LEU:HD21	1:A:1132:PRO:HD2	1.98	0.44
1:A:232:MET:HB3	1:A:282:LEU:HD13	2.00	0.44
8:A:2021:Y01:HAE1	8:A:2021:Y01:CAD	2.48	0.44
1:A:602:ALA:HB1	1:A:607:THR:HG21	2.00	0.43
9:A:2006:3PE:H3C1	8:A:2020:Y01:HAB2	2.00	0.43
1:A:1849:ASN:OD1	1:A:1849:ASN:O	2.36	0.43
1:A:340:LEU:O	1:A:340:LEU:HD23	2.18	0.43
2:E:97:LEU:HD11	2:E:152:VAL:HG21	2.00	0.43
1:A:687:LEU:HD11	1:A:1358:TYR:CE1	2.54	0.43
1:A:1819:ALA:HB3	8:A:2020:Y01:HAR1	2.01	0.43
9:A:2006:3PE:H3A2	8:A:2028:Y01:HBA	2.00	0.43
8:A:2005:Y01:HAT2	8:A:2005:Y01:HAS2	1.41	0.43
8:A:2020:Y01:HAS2	8:A:2020:Y01:HAT2	1.61	0.43
8:A:2023:Y01:HAD2	8:A:2023:Y01:HAS2	1.89	0.43
8:H:102:Y01:HAM2	8:H:102:Y01:HBC	1.61	0.43
1:A:992:LYS:HG3	1:A:993:MET:N	2.34	0.43
1:A:1602:ILE:O	1:A:1606:THR:HG22	2.18	0.43
8:A:2005:Y01:HAA1	8:A:2005:Y01:HAP1	2.00	0.43
8:A:2017:Y01:HAA2	8:A:2017:Y01:HAJ2	1.85	0.43
1:A:582:ILE:O	1:A:1284:VAL:CG2	2.67	0.42
8:A:2017:Y01:HAS2	8:A:2017:Y01:HAT2	1.52	0.42
8:A:2025:Y01:HAE2	8:A:2025:Y01:HBB	1.74	0.42
8:A:2011:Y01:HAD3	8:A:2011:Y01:HBD	1.81	0.42
8:A:2015:Y01:HAP1	8:A:2015:Y01:HAO2	1.20	0.42
8:A:2019:Y01:HAE2	8:A:2019:Y01:HBB	1.68	0.42
1:A:1159:SER:HB2	1:A:1250:LEU:HD21	2.00	0.42
1:A:1644:GLY:HA3	8:A:2026:Y01:HAS1	2.02	0.42
8:A:2008:Y01:HAS2	8:A:2008:Y01:HAD2	1.65	0.42
8:A:2016:Y01:HAS2	8:A:2016:Y01:HAT2	1.60	0.42
1:A:550:PHE:CE1	8:A:2012:Y01:HAK2	2.54	0.42
8:A:2018:Y01:HAS2	8:A:2018:Y01:HAT2	1.61	0.42
1:A:954:ILE:CD1	1:A:1021:LEU:HD23	2.49	0.42
8:A:2026:Y01:HAS2	8:A:2026:Y01:HAT2	1.64	0.42
1:A:462:ILE:CD1	8:A:2003:Y01:HAD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2014:Y01:HAB2	8:A:2014:Y01:HAJ2	1.84	0.42
1:A:449:VAL:HG22	8:A:2013:Y01:HAC3	2.01	0.42
1:A:949:THR:HG23	1:A:952:ARG:H	1.85	0.42
8:A:2005:Y01:HAE1	8:A:2005:Y01:HBD	1.88	0.42
8:A:2007:Y01:CAC	8:A:2010:Y01:HAK2	2.50	0.42
8:A:2021:Y01:HAC1	8:A:2021:Y01:HAU2	2.02	0.42
8:A:2024:Y01:HAS2	8:A:2024:Y01:HAD2	1.81	0.42
4:H:3:THR:HG21	8:H:102:Y01:HAL1	2.01	0.42
8:A:2029:Y01:HAB2	8:A:2029:Y01:HAJ1	1.80	0.42
1:A:524:GLY:HA2	1:A:601:VAL:HA	2.02	0.42
1:A:1819:ALA:HB1	8:A:2020:Y01:HAR1	2.02	0.42
8:A:2002:Y01:HAC2	8:A:2011:Y01:HAA3	2.02	0.41
1:A:1107:ASN:ND2	1:A:1112:CYS:SG	2.93	0.41
8:A:2009:Y01:HAD3	8:A:2009:Y01:HBD	1.87	0.41
8:A:2017:Y01:HBD	8:A:2017:Y01:HAD3	1.80	0.41
8:A:2030:Y01:HAD2	8:A:2030:Y01:HAS2	1.79	0.41
8:A:2015:Y01:HAC2	8:A:2015:Y01:HAJ2	1.61	0.41
8:A:2027:Y01:HAP1	8:A:2027:Y01:HAO1	1.53	0.41
1:A:639:PHE:CZ	8:H:102:Y01:HAR1	2.55	0.41
1:A:1291:TYR:O	1:A:1295:PRO:HD2	2.21	0.41
1:A:1364:ILE:HG22	1:A:1368:ILE:HD12	2.02	0.41
1:A:1526:VAL:HG11	1:A:1736:GLU:HG2	2.01	0.41
8:A:2007:Y01:HAU2	8:A:2007:Y01:CAC	2.51	0.41
8:A:2012:Y01:HAS1	8:A:2012:Y01:HAT1	1.57	0.41
1:A:671:VAL:O	1:A:671:VAL:CG1	2.67	0.41
8:A:2002:Y01:HAS2	8:A:2002:Y01:HAT2	1.75	0.41
8:A:2018:Y01:HAC2	8:A:2018:Y01:HAJ2	1.65	0.41
1:A:1365:VAL:HG21	5:D:9:BGC:C1	2.51	0.41
8:A:2002:Y01:HAO2	8:A:2002:Y01:HAP1	1.39	0.41
8:A:2005:Y01:HAA1	8:A:2005:Y01:HAJ2	1.81	0.41
8:A:2011:Y01:HAS2	8:A:2011:Y01:HAT2	1.72	0.41
8:A:2022:Y01:OAG	8:A:2022:Y01:HAV2	2.21	0.41
8:A:2002:Y01:HAC2	8:A:2002:Y01:HAJ2	1.64	0.41
8:A:2003:Y01:HAA2	8:A:2003:Y01:HAJ1	1.83	0.41
8:A:2030:Y01:HAS2	8:A:2030:Y01:HAT2	1.66	0.41
1:A:590:THR:O	1:A:590:THR:HG23	2.21	0.41
1:A:852:ARG:NH1	1:A:859:GLU:OE2	2.54	0.41
8:A:2003:Y01:HAR1	8:A:2024:Y01:HAP2	2.02	0.41
8:A:2003:Y01:HAD2	8:A:2003:Y01:HAS2	1.67	0.41
8:A:2028:Y01:HAD3	8:A:2028:Y01:HBD	1.75	0.41
1:A:1522:TRP:CZ2	1:A:1526:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2020:Y01:HAJ2	8:A:2020:Y01:HAC2	1.63	0.41
8:A:2026:Y01:HAS2	8:A:2026:Y01:HAD2	1.84	0.41
1:A:1465:VAL:HG12	1:A:1670:VAL:HG22	2.01	0.41
8:A:2019:Y01:HAS2	8:A:2019:Y01:HAD2	1.80	0.41
1:A:1285:ASP:OD1	1:A:1285:ASP:N	2.53	0.40
1:A:1462:PHE:CA	1:A:1673:LEU:HD23	2.52	0.40
8:A:2002:Y01:HAE2	8:A:2002:Y01:HBB	1.74	0.40
8:A:2009:Y01:HAA2	8:A:2009:Y01:HAJ2	1.77	0.40
8:A:2025:Y01:HAJ2	8:A:2025:Y01:HAC2	1.66	0.40
8:A:2030:Y01:HAC1	8:A:2030:Y01:HAU2	2.03	0.40
2:E:26:LEU:CD1	2:E:172:VAL:HG22	2.52	0.40
1:A:1195:HIS:CB	1:A:1196:PRO:HD3	2.51	0.40
8:A:2008:Y01:HAP2	8:A:2018:Y01:HAD2	2.02	0.40
8:A:2010:Y01:HAS1	8:A:2013:Y01:HAU1	2.04	0.40
8:A:2012:Y01:HAD3	8:A:2012:Y01:HBD	1.89	0.40
8:A:2014:Y01:HAI	8:A:2029:Y01:HAD1	2.02	0.40
1:A:853:ILE:CG2	1:A:1021:LEU:CD1	3.00	0.40
8:A:2027:Y01:HAE2	8:A:2027:Y01:HBB	1.72	0.40
1:A:182:MET:HE3	3:G:105:PRO:HG3	2.04	0.40
8:A:2025:Y01:HBFB	8:A:2026:Y01:CAD	2.51	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	1663/1931 (86%)	1636 (98%)	27 (2%)	0	100	100
2	E	177/235 (75%)	174 (98%)	3 (2%)	0	100	100
3	G	70/197 (36%)	65 (93%)	5 (7%)	0	100	100
4	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1911/2369 (81%)	1876 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1400/1663 (84%)	1393 (100%)	7 (0%)	81	85
2	E	130/203 (64%)	130 (100%)	0	100	100
3	G	60/167 (36%)	60 (100%)	0	100	100
4	H	1/1 (100%)	0	1 (100%)	0	0
All	All	1591/2034 (78%)	1583 (100%)	8 (0%)	78	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	684	ASP
1	A	694	LEU
1	A	1088	HIS
1	A	1133	TYR
1	A	1195	HIS
1	A	1658	PHE
4	H	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	188	HIS
1	A	317	GLN
1	A	771	HIS
1	A	778	HIS
1	A	948	GLN
1	A	972	ASN
1	A	1243	GLN
1	A	1469	GLN

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Mol	Chain	Res	Type
1	A	1514	ASN
1	A	1559	ASN
1	A	1688	HIS
1	A	1701	ASN
1	A	1779	GLN
2	E	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	A1CHU	H	6	4	6,8,9	0.43	0	4,9,11	1.06	1 (25%)
4	HYP	H	4	4	7,8,9	0.49	0	5,10,12	0.97	1 (20%)
4	HY3	H	7	4	7,8,9	0.70	0	7,10,12	0.78	0
4	A1CHT	H	5	4	14,15,16	0.32	0	16,20,22	0.54	0
4	A1CHS	H	2	12,4	8,12,13	0.74	0	8,14,16	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1CHU	H	6	4	-	5/8/9/11	-
4	HYP	H	4	4	-	0/0/11/13	0/1/1/1
4	HY3	H	7	4	-	0/1/12/14	0/1/1/1
4	A1CHT	H	5	4	-	2/13/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1CHS	H	2	12,4	-	7/11/14/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6	A1CHU	O-C-CA	-2.09	119.40	124.77
4	H	4	HYP	O-C-CA	-2.08	119.41	124.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	A1CHS	O-C-CA-CB
4	H	2	A1CHS	N-CA-CB-CG
4	H	2	A1CHS	N19-CD-CG-CB
4	H	2	A1CHS	N19-CD-CG-O58
4	H	2	A1CHS	NE-CD-CG-O58
4	H	6	A1CHU	O-C-CA-CB
4	H	6	A1CHU	C-CA-CB-CG
4	H	6	A1CHU	C-CA-CB-O36
4	H	6	A1CHU	N-CA-CB-CG
4	H	6	A1CHU	N-CA-CB-O36
4	H	2	A1CHS	N19-C20-C21-N22
4	H	5	A1CHT	N-CA-CB-CG2
4	H	2	A1CHS	C21-C20-N19-CD
4	H	5	A1CHT	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

22 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	BGC	D	1	5	12,12,12	1.25	1 (8%)	17,17,17	0.64	0
5	BGC	D	10	5	11,11,12	1.67	2 (18%)	15,15,17	0.85	1 (6%)
5	BGC	D	11	5	11,11,12	1.68	3 (27%)	15,15,17	0.85	0
5	BGC	D	12	5	11,11,12	1.62	2 (18%)	15,15,17	1.17	1 (6%)
5	BGC	D	13	5	11,11,12	1.69	2 (18%)	15,15,17	0.82	0
5	BGC	D	14	5	11,11,12	1.64	2 (18%)	15,15,17	0.86	0
5	BGC	D	15	5	11,11,12	1.51	2 (18%)	15,15,17	1.69	4 (26%)
5	BGC	D	16	5	11,11,12	1.61	2 (18%)	15,15,17	1.03	1 (6%)
5	BGC	D	17	5	11,11,12	1.65	2 (18%)	15,15,17	1.41	1 (6%)
5	BGC	D	2	5	11,11,12	1.58	2 (18%)	15,15,17	0.95	1 (6%)
5	BGC	D	3	5	11,11,12	1.60	2 (18%)	15,15,17	1.21	1 (6%)
5	BGC	D	4	5	11,11,12	1.63	2 (18%)	15,15,17	0.99	1 (6%)
5	BGC	D	5	5	11,11,12	1.60	2 (18%)	15,15,17	1.13	1 (6%)
5	BGC	D	6	5	11,11,12	1.62	2 (18%)	15,15,17	1.28	1 (6%)
5	BGC	D	7	5	11,11,12	1.57	2 (18%)	15,15,17	1.14	1 (6%)
5	BGC	D	8	5	11,11,12	1.56	2 (18%)	15,15,17	1.05	0
5	BGC	D	9	5	11,11,12	1.61	3 (27%)	15,15,17	0.74	0
6	NAG	K	1	6,1	14,14,15	0.42	0	17,19,21	0.71	0
6	NAG	K	2	6	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
6	BMA	K	3	6	11,11,12	0.25	0	15,15,17	0.69	0
6	MAN	K	4	6	11,11,12	0.24	0	15,15,17	0.84	1 (6%)
6	MAN	K	5	6	11,11,12	0.28	0	15,15,17	0.56	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	BGC	D	1	5	-	0/2/22/22	0/1/1/1
5	BGC	D	10	5	-	0/2/19/22	0/1/1/1
5	BGC	D	11	5	-	0/2/19/22	0/1/1/1
5	BGC	D	12	5	-	0/2/19/22	0/1/1/1
5	BGC	D	13	5	-	0/2/19/22	0/1/1/1
5	BGC	D	14	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BGC	D	15	5	-	0/2/19/22	0/1/1/1
5	BGC	D	16	5	-	0/2/19/22	0/1/1/1
5	BGC	D	17	5	-	1/2/19/22	0/1/1/1
5	BGC	D	2	5	-	0/2/19/22	0/1/1/1
5	BGC	D	3	5	-	0/2/19/22	0/1/1/1
5	BGC	D	4	5	-	1/2/19/22	0/1/1/1
5	BGC	D	5	5	-	1/2/19/22	0/1/1/1
5	BGC	D	6	5	-	0/2/19/22	0/1/1/1
5	BGC	D	7	5	-	1/2/19/22	0/1/1/1
5	BGC	D	8	5	-	0/2/19/22	0/1/1/1
5	BGC	D	9	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	10	BGC	O5-C1	4.24	1.50	1.43
5	D	17	BGC	O5-C1	4.24	1.50	1.43
5	D	11	BGC	O5-C1	4.13	1.50	1.43
5	D	13	BGC	O5-C1	4.13	1.50	1.43
5	D	14	BGC	O5-C1	4.12	1.50	1.43
5	D	4	BGC	O5-C1	4.03	1.50	1.43
5	D	3	BGC	O5-C1	4.03	1.50	1.43
5	D	12	BGC	O5-C1	4.00	1.50	1.43
5	D	16	BGC	O5-C1	4.00	1.50	1.43
5	D	2	BGC	O5-C1	3.97	1.50	1.43
5	D	5	BGC	O5-C1	3.94	1.50	1.43
5	D	7	BGC	O5-C1	3.93	1.50	1.43
5	D	6	BGC	O5-C1	3.92	1.50	1.43
5	D	9	BGC	O5-C1	3.84	1.50	1.43
5	D	8	BGC	O5-C1	3.80	1.50	1.43
5	D	15	BGC	O5-C1	3.79	1.50	1.43
5	D	1	BGC	O5-C1	3.26	1.50	1.42
5	D	13	BGC	C2-C3	-2.75	1.48	1.52
5	D	6	BGC	C2-C3	-2.69	1.48	1.52
5	D	11	BGC	C2-C3	-2.61	1.48	1.52
5	D	5	BGC	C2-C3	-2.56	1.48	1.52
5	D	12	BGC	C2-C3	-2.55	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	9	BGC	C2-C3	-2.55	1.48	1.52
5	D	14	BGC	C2-C3	-2.54	1.48	1.52
5	D	16	BGC	C2-C3	-2.47	1.48	1.52
5	D	4	BGC	C2-C3	-2.47	1.48	1.52
5	D	10	BGC	C2-C3	-2.41	1.48	1.52
5	D	7	BGC	C2-C3	-2.37	1.48	1.52
5	D	3	BGC	C2-C3	-2.36	1.48	1.52
5	D	2	BGC	C2-C3	-2.35	1.48	1.52
5	D	17	BGC	C2-C3	-2.30	1.49	1.52
5	D	15	BGC	C2-C3	-2.24	1.49	1.52
5	D	8	BGC	C2-C3	-2.17	1.49	1.52
5	D	11	BGC	O5-C5	2.15	1.47	1.43
5	D	9	BGC	O5-C5	2.07	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	17	BGC	C1-C2-C3	4.27	115.86	109.64
5	D	15	BGC	C1-C2-C3	4.07	115.57	109.64
5	D	3	BGC	C1-C2-C3	3.27	114.41	109.64
5	D	7	BGC	C1-C2-C3	3.26	114.38	109.64
5	D	12	BGC	C1-C2-C3	3.03	114.06	109.64
5	D	16	BGC	C1-C2-C3	2.97	113.97	109.64
6	K	2	NAG	C2-N2-C7	2.86	126.73	122.90
5	D	6	BGC	C1-C2-C3	2.85	113.80	109.64
5	D	2	BGC	C1-O5-C5	-2.74	108.51	112.19
5	D	15	BGC	C2-C3-C4	2.68	115.57	110.86
5	D	4	BGC	C1-C2-C3	2.43	113.17	109.64
5	D	15	BGC	C3-C4-C5	2.29	114.39	110.23
5	D	15	BGC	O3-C3-C2	-2.29	105.39	110.05
5	D	5	BGC	C1-C2-C3	2.15	112.78	109.64
5	D	10	BGC	C1-C2-C3	2.08	112.67	109.64
6	K	4	MAN	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	D	4	BGC	O5-C5-C6-O6
5	D	7	BGC	O5-C5-C6-O6

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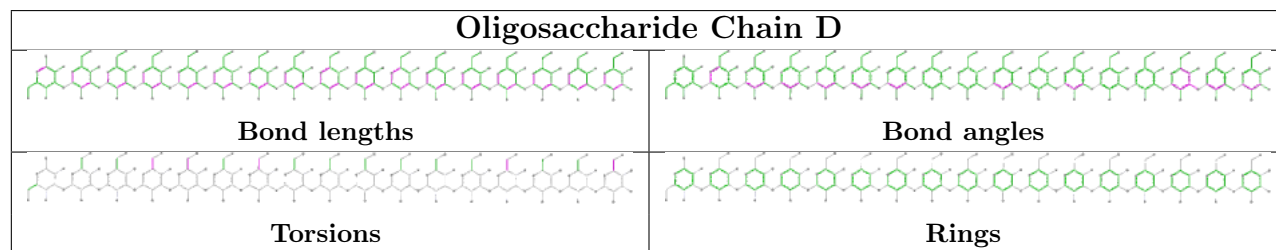
Mol	Chain	Res	Type	Atoms
5	D	5	BGC	O5-C5-C6-O6
5	D	17	BGC	O5-C5-C6-O6
6	K	1	NAG	C3-C2-N2-C7
5	D	14	BGC	O5-C5-C6-O6

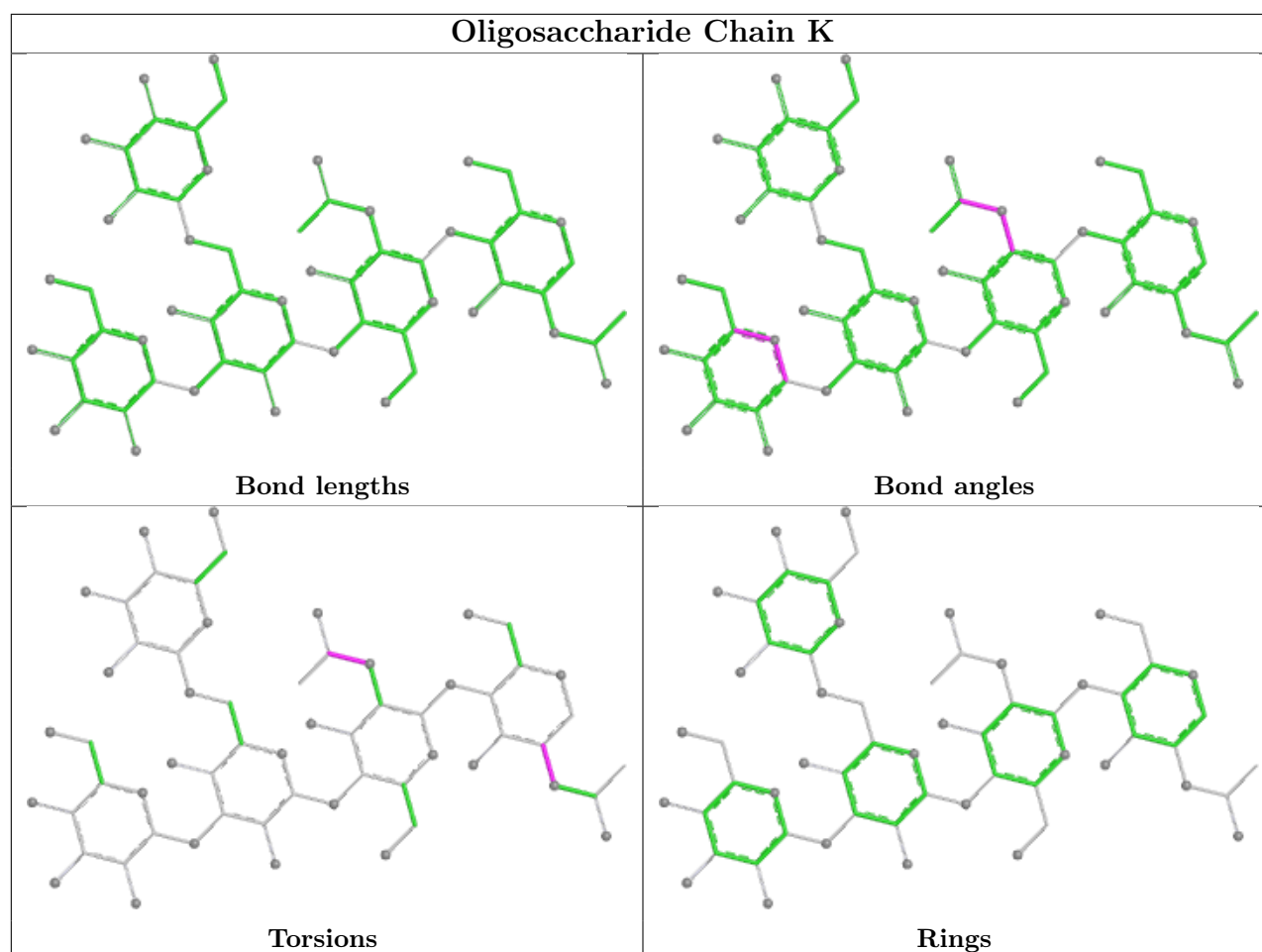
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	10	BGC	1	0
5	D	15	BGC	1	0
5	D	9	BGC	2	0
5	D	16	BGC	1	0

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





5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
8	Y01	A	2011	-	38,38,38	1.09	3 (7%)	57,57,57	3.13	17 (29%)
8	Y01	A	2030	-	38,38,38	1.08	3 (7%)	57,57,57	3.25	20 (35%)
11	GSP	E	301	-	33,34,34	3.29	18 (54%)	47,54,54	2.16	11 (23%)
8	Y01	A	2016	-	38,38,38	1.08	3 (7%)	57,57,57	3.22	19 (33%)
8	Y01	A	2003	-	38,38,38	1.07	3 (7%)	57,57,57	3.15	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	Y01	A	2021	-	38,38,38	1.09	3 (7%)	57,57,57	3.31	20 (35%)
8	Y01	A	2029	-	38,38,38	1.10	3 (7%)	57,57,57	3.35	19 (33%)
12	A1CHR	H	101	4	15,16,17	0.15	0	16,17,19	0.37	0
8	Y01	A	2004	-	38,38,38	1.10	3 (7%)	57,57,57	3.34	18 (31%)
8	Y01	A	2019	-	38,38,38	1.08	3 (7%)	57,57,57	3.21	19 (33%)
8	Y01	A	2027	-	38,38,38	1.07	3 (7%)	57,57,57	3.13	18 (31%)
8	Y01	A	2026	-	38,38,38	1.09	3 (7%)	57,57,57	3.25	18 (31%)
9	3PE	A	2006	-	48,48,50	0.48	0	51,53,55	0.45	0
8	Y01	A	2009	-	38,38,38	1.09	3 (7%)	57,57,57	3.34	19 (33%)
8	Y01	A	2024	-	38,38,38	1.08	3 (7%)	57,57,57	3.17	20 (35%)
8	Y01	A	2020	-	38,38,38	1.08	3 (7%)	57,57,57	3.26	17 (29%)
8	Y01	A	2015	-	38,38,38	1.09	3 (7%)	57,57,57	3.30	19 (33%)
8	Y01	A	2008	-	38,38,38	1.08	3 (7%)	57,57,57	3.41	23 (40%)
7	NAG	A	2001	1	14,14,15	0.21	0	17,19,21	0.42	0
8	Y01	A	2017	-	38,38,38	1.09	3 (7%)	57,57,57	3.26	18 (31%)
8	Y01	A	2010	-	38,38,38	1.08	3 (7%)	57,57,57	3.20	18 (31%)
8	Y01	A	2002	-	38,38,38	1.06	3 (7%)	57,57,57	3.14	19 (33%)
8	Y01	A	2022	-	38,38,38	1.07	3 (7%)	57,57,57	3.20	18 (31%)
8	Y01	A	2028	-	38,38,38	1.08	3 (7%)	57,57,57	3.12	15 (26%)
8	Y01	A	2013	-	38,38,38	1.07	3 (7%)	57,57,57	3.32	20 (35%)
8	Y01	A	2007	-	38,38,38	1.10	3 (7%)	57,57,57	3.23	20 (35%)
8	Y01	A	2012	-	38,38,38	1.08	3 (7%)	57,57,57	3.28	20 (35%)
8	Y01	H	102	-	38,38,38	1.07	3 (7%)	57,57,57	3.20	17 (29%)
8	Y01	A	2014	-	38,38,38	1.08	3 (7%)	57,57,57	3.28	22 (38%)
8	Y01	A	2025	-	38,38,38	1.07	3 (7%)	57,57,57	3.19	18 (31%)
8	Y01	A	2023	-	38,38,38	1.06	3 (7%)	57,57,57	3.10	16 (28%)
8	Y01	A	2018	-	38,38,38	1.07	3 (7%)	57,57,57	3.19	19 (33%)
8	Y01	A	2005	-	38,38,38	1.10	3 (7%)	57,57,57	3.37	19 (33%)
10	UDP	A	2031	-	25,26,26	3.80	14 (56%)	38,40,40	1.57	5 (13%)

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
8	Y01	A	2011	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2030	-	-	9/19/77/77	0/4/4/4
11	GSP	E	301	-	-	6/21/38/38	0/3/3/3
8	Y01	A	2016	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2003	-	-	13/19/77/77	0/4/4/4
8	Y01	A	2021	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2029	-	-	9/19/77/77	0/4/4/4
12	A1CHR	H	101	4	-	6/16/16/17	-
8	Y01	A	2004	-	-	6/19/77/77	0/4/4/4
8	Y01	A	2019	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2027	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2026	-	-	15/19/77/77	0/4/4/4
9	3PE	A	2006	-	-	21/52/52/54	-
8	Y01	A	2009	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2024	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2020	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2015	-	-	15/19/77/77	0/4/4/4
8	Y01	A	2008	-	-	10/19/77/77	0/4/4/4
7	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
8	Y01	A	2017	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2010	-	-	8/19/77/77	0/4/4/4
8	Y01	A	2002	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2022	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2028	-	-	7/19/77/77	0/4/4/4
8	Y01	A	2013	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2007	-	-	8/19/77/77	0/4/4/4
8	Y01	A	2012	-	-	9/19/77/77	0/4/4/4
8	Y01	H	102	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2014	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2025	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2023	-	-	14/19/77/77	0/4/4/4
8	Y01	A	2018	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2005	-	-	7/19/77/77	0/4/4/4
10	UDP	A	2031	-	-	3/16/32/32	0/2/2/2

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2031	UDP	O4'-C4'	7.41	1.61	1.45
10	A	2031	UDP	C3'-C4'	-7.25	1.34	1.53
10	A	2031	UDP	C2-N1	6.86	1.49	1.38
11	E	301	GSP	C4-N3	6.61	1.49	1.34
10	A	2031	UDP	C2-N3	6.60	1.49	1.38
11	E	301	GSP	O4'-C4'	-6.33	1.30	1.45
10	A	2031	UDP	C6-C5	6.02	1.49	1.35
10	A	2031	UDP	PA-O3A	5.51	1.65	1.59
11	E	301	GSP	C1'-N9	-5.45	1.32	1.47
11	E	301	GSP	C2-N3	5.29	1.46	1.33
11	E	301	GSP	PB-O3B	5.26	1.65	1.59
10	A	2031	UDP	O4'-C1'	-5.26	1.29	1.42
11	E	301	GSP	C3'-C4'	5.05	1.65	1.53
11	E	301	GSP	C2-N2	4.70	1.45	1.34
11	E	301	GSP	O4'-C1'	4.34	1.52	1.42
11	E	301	GSP	PB-O3A	4.33	1.64	1.59
11	E	301	GSP	PA-O3A	4.12	1.64	1.59
10	A	2031	UDP	C4-N3	4.04	1.45	1.38
11	E	301	GSP	C5-N7	-3.55	1.32	1.39
11	E	301	GSP	PG-O3G	3.47	1.66	1.54
8	A	2011	Y01	OAW-CAY	3.35	1.43	1.34
8	A	2012	Y01	OAW-CAY	3.32	1.43	1.34
8	A	2019	Y01	OAW-CAY	3.30	1.43	1.34
8	A	2008	Y01	OAW-CAY	3.30	1.43	1.34
8	A	2024	Y01	OAW-CAY	3.29	1.43	1.34
8	A	2021	Y01	OAW-CAY	3.27	1.43	1.34
8	A	2026	Y01	OAW-CAY	3.27	1.43	1.34
8	A	2007	Y01	OAW-CAY	3.26	1.43	1.34
8	A	2030	Y01	OAW-CAY	3.26	1.43	1.34
8	A	2017	Y01	OAW-CAY	3.25	1.43	1.34
8	A	2022	Y01	OAW-CAY	3.25	1.43	1.34
8	A	2014	Y01	OAW-CAY	3.25	1.43	1.34
8	A	2015	Y01	OAW-CAY	3.25	1.43	1.34
8	A	2027	Y01	OAW-CAY	3.24	1.43	1.34
8	A	2004	Y01	OAW-CAY	3.24	1.43	1.34
8	A	2016	Y01	OAW-CAY	3.24	1.43	1.34
8	A	2028	Y01	OAW-CAY	3.24	1.43	1.34
8	A	2018	Y01	OAW-CAY	3.24	1.43	1.34
8	A	2009	Y01	OAW-CAY	3.23	1.43	1.34
8	A	2005	Y01	OAW-CAY	3.23	1.43	1.34
8	A	2020	Y01	OAW-CAY	3.23	1.43	1.34
8	A	2003	Y01	OAW-CAY	3.22	1.43	1.34
8	H	102	Y01	OAW-CAY	3.22	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2029	Y01	OAW-CAY	3.21	1.43	1.34
8	A	2010	Y01	OAW-CAY	3.20	1.43	1.34
8	A	2025	Y01	OAW-CAY	3.19	1.43	1.34
8	A	2002	Y01	OAW-CAY	3.19	1.43	1.34
8	A	2023	Y01	OAW-CAY	3.17	1.43	1.34
8	A	2013	Y01	OAW-CAY	3.16	1.43	1.34
11	E	301	GSP	PG-O2G	3.13	1.64	1.54
10	A	2031	UDP	C6-N1	3.06	1.45	1.38
10	A	2031	UDP	O4-C4	-2.93	1.18	1.24
11	E	301	GSP	O2'-C2'	2.88	1.50	1.43
8	A	2010	Y01	OAH-CAX	-2.87	1.21	1.30
8	A	2003	Y01	OAH-CAX	-2.87	1.21	1.30
8	H	102	Y01	OAH-CAX	-2.87	1.21	1.30
8	A	2026	Y01	OAH-CAX	-2.86	1.21	1.30
8	A	2016	Y01	OAH-CAX	-2.86	1.21	1.30
8	A	2014	Y01	OAH-CAX	-2.86	1.21	1.30
8	A	2002	Y01	OAH-CAX	-2.86	1.21	1.30
8	A	2024	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2027	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2028	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2029	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2025	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2030	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2005	Y01	OAH-CAX	-2.85	1.21	1.30
8	A	2004	Y01	OAH-CAX	-2.84	1.21	1.30
8	A	2022	Y01	OAH-CAX	-2.84	1.21	1.30
8	A	2021	Y01	OAH-CAX	-2.84	1.21	1.30
8	A	2015	Y01	OAH-CAX	-2.84	1.21	1.30
8	A	2018	Y01	OAH-CAX	-2.84	1.21	1.30
8	A	2017	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2008	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2023	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2013	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2012	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2009	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2020	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2011	Y01	OAH-CAX	-2.83	1.21	1.30
8	A	2019	Y01	OAH-CAX	-2.82	1.21	1.30
8	A	2007	Y01	OAH-CAX	-2.82	1.21	1.30
11	E	301	GSP	O6-C6	-2.79	1.18	1.23
10	A	2031	UDP	O2'-C2'	-2.68	1.36	1.43
10	A	2031	UDP	O3'-C3'	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	301	GSP	C2-N1	2.51	1.43	1.37
10	A	2031	UDP	O2-C2	-2.46	1.18	1.23
8	A	2011	Y01	CAK-CAI	2.43	1.55	1.50
8	A	2028	Y01	CAK-CAI	2.41	1.55	1.50
10	A	2031	UDP	C5-C4	2.41	1.48	1.43
8	A	2007	Y01	CAK-CAI	2.39	1.55	1.50
8	A	2004	Y01	CAK-CAI	2.35	1.55	1.50
8	A	2020	Y01	CAK-CAI	2.34	1.55	1.50
8	A	2017	Y01	CAK-CAI	2.31	1.54	1.50
8	H	102	Y01	CAK-CAI	2.30	1.54	1.50
8	A	2005	Y01	CAK-CAI	2.30	1.54	1.50
8	A	2013	Y01	CAK-CAI	2.29	1.54	1.50
8	A	2010	Y01	CAK-CAI	2.29	1.54	1.50
8	A	2029	Y01	CAK-CAI	2.28	1.54	1.50
8	A	2009	Y01	CAK-CAI	2.28	1.54	1.50
8	A	2016	Y01	CAK-CAI	2.27	1.54	1.50
8	A	2002	Y01	CAK-CAI	2.23	1.54	1.50
8	A	2018	Y01	CAK-CAI	2.21	1.54	1.50
8	A	2015	Y01	CAK-CAI	2.21	1.54	1.50
8	A	2012	Y01	CAK-CAI	2.20	1.54	1.50
8	A	2023	Y01	CAK-CAI	2.19	1.54	1.50
8	A	2014	Y01	CAK-CAI	2.19	1.54	1.50
8	A	2025	Y01	CAK-CAI	2.19	1.54	1.50
8	A	2021	Y01	CAK-CAI	2.18	1.54	1.50
8	A	2030	Y01	CAK-CAI	2.16	1.54	1.50
8	A	2027	Y01	CAK-CAI	2.16	1.54	1.50
8	A	2024	Y01	CAK-CAI	2.15	1.54	1.50
11	E	301	GSP	C5-C6	2.14	1.52	1.44
8	A	2026	Y01	CAK-CAI	2.13	1.54	1.50
11	E	301	GSP	C6-N1	2.08	1.42	1.38
8	A	2019	Y01	CAK-CAI	2.06	1.54	1.50
8	A	2022	Y01	CAK-CAI	2.06	1.54	1.50
8	A	2003	Y01	CAK-CAI	2.05	1.54	1.50
8	A	2008	Y01	CAK-CAI	2.01	1.54	1.50

All (562) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2027	Y01	CAT-CBH-CBF	-14.52	89.52	108.74
8	A	2020	Y01	CAT-CBH-CBF	-14.51	89.54	108.74
8	A	2023	Y01	CAT-CBH-CBF	-14.44	89.64	108.74
8	A	2002	Y01	CAT-CBH-CBF	-14.35	89.74	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2016	Y01	CAT-CBH-CBF	-14.24	89.89	108.74
8	A	2015	Y01	CAT-CBH-CBF	-14.17	89.98	108.74
8	A	2022	Y01	CAT-CBH-CBF	-14.14	90.03	108.74
8	A	2024	Y01	CAT-CBH-CBF	-14.12	90.06	108.74
8	A	2025	Y01	CAT-CBH-CBF	-14.07	90.12	108.74
8	A	2003	Y01	CAT-CBH-CBF	-14.05	90.15	108.74
8	A	2017	Y01	CAT-CBH-CBF	-13.99	90.22	108.74
8	A	2014	Y01	CAT-CBH-CBF	-13.99	90.23	108.74
8	A	2026	Y01	CAT-CBH-CBF	-13.98	90.23	108.74
8	A	2010	Y01	CAT-CBH-CBF	-13.97	90.25	108.74
8	A	2021	Y01	CAT-CBH-CBF	-13.89	90.36	108.74
8	A	2030	Y01	CAT-CBH-CBF	-13.87	90.39	108.74
8	A	2009	Y01	CAT-CBH-CBF	-13.87	90.39	108.74
8	A	2019	Y01	CAT-CBH-CBF	-13.82	90.45	108.74
8	A	2005	Y01	CAT-CBH-CBF	-13.80	90.48	108.74
8	A	2018	Y01	CAT-CBH-CBF	-13.75	90.54	108.74
8	A	2028	Y01	CAT-CBH-CBF	-13.74	90.56	108.74
8	A	2029	Y01	CAT-CBH-CBF	-13.73	90.56	108.74
8	A	2011	Y01	CAT-CBH-CBF	-13.72	90.58	108.74
8	A	2008	Y01	CAT-CBH-CBF	-13.68	90.64	108.74
8	A	2012	Y01	CAT-CBH-CBF	-13.59	90.75	108.74
8	A	2004	Y01	CAT-CBH-CBF	-13.39	91.02	108.74
8	A	2007	Y01	CAT-CBH-CBF	-13.22	91.24	108.74
8	A	2013	Y01	CAT-CBH-CBF	-12.61	92.05	108.74
8	H	102	Y01	CAT-CBH-CBF	-12.53	92.16	108.74
8	H	102	Y01	CAV-CAZ-CAI	10.45	134.74	120.57
8	A	2013	Y01	CAV-CAZ-CAI	10.18	134.37	120.57
8	A	2007	Y01	CAV-CAZ-CAI	9.47	133.41	120.57
8	A	2012	Y01	CAV-CAZ-CAI	9.38	133.29	120.57
8	A	2008	Y01	CAV-CAZ-CAI	9.26	133.13	120.57
8	A	2020	Y01	CAV-CAZ-CAI	9.25	133.11	120.57
8	A	2005	Y01	CAV-CAZ-CAI	9.24	133.09	120.57
8	A	2029	Y01	CAV-CAZ-CAI	9.15	132.97	120.57
8	A	2009	Y01	CAV-CAZ-CAI	9.14	132.95	120.57
8	A	2022	Y01	CAV-CAZ-CAI	9.12	132.93	120.57
8	A	2030	Y01	CAV-CAZ-CAI	9.11	132.91	120.57
8	A	2004	Y01	CAV-CAZ-CAI	9.10	132.91	120.57
8	A	2028	Y01	CAV-CAZ-CAI	9.05	132.83	120.57
8	A	2015	Y01	CAV-CAZ-CAI	9.03	132.81	120.57
8	A	2017	Y01	CAV-CAZ-CAI	9.02	132.80	120.57
8	A	2016	Y01	CAV-CAZ-CAI	9.00	132.77	120.57
8	A	2026	Y01	CAV-CAZ-CAI	9.00	132.77	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2021	Y01	CAV-CAZ-CAI	8.98	132.74	120.57
8	A	2019	Y01	CAV-CAZ-CAI	8.98	132.74	120.57
8	A	2014	Y01	CAV-CAZ-CAI	8.95	132.70	120.57
8	A	2003	Y01	CAV-CAZ-CAI	8.94	132.68	120.57
8	A	2010	Y01	CAV-CAZ-CAI	8.93	132.68	120.57
8	A	2011	Y01	CAV-CAZ-CAI	8.91	132.65	120.57
8	A	2025	Y01	CAV-CAZ-CAI	8.91	132.65	120.57
8	A	2023	Y01	CAV-CAZ-CAI	8.91	132.64	120.57
8	A	2024	Y01	CAV-CAZ-CAI	8.82	132.53	120.57
8	A	2002	Y01	CAV-CAZ-CAI	8.81	132.52	120.57
8	A	2018	Y01	CAV-CAZ-CAI	8.67	132.33	120.57
8	A	2027	Y01	CAV-CAZ-CAI	8.63	132.26	120.57
8	A	2013	Y01	CBH-CAZ-CAI	-8.39	110.68	122.93
8	A	2004	Y01	CBH-CAZ-CAI	-8.19	110.97	122.93
8	H	102	Y01	CBH-CAZ-CAI	-7.57	111.87	122.93
8	A	2029	Y01	CBH-CBF-CBD	-7.37	101.94	112.71
8	A	2009	Y01	CBH-CBF-CBD	-7.36	101.95	112.71
8	A	2011	Y01	CBH-CAZ-CAI	-7.36	112.19	122.93
8	A	2018	Y01	CBH-CBF-CBD	-7.23	102.15	112.71
8	A	2017	Y01	CBH-CBF-CBD	-7.15	102.26	112.71
8	A	2012	Y01	CBH-CBF-CBD	-7.03	102.44	112.71
8	A	2007	Y01	CBH-CAZ-CAI	-6.97	112.75	122.93
8	A	2010	Y01	CBH-CBF-CBD	-6.96	102.55	112.71
8	A	2005	Y01	CBH-CBF-CBD	-6.92	102.60	112.71
8	A	2028	Y01	CBH-CAZ-CAI	-6.88	112.89	122.93
8	A	2028	Y01	CBH-CBF-CBD	-6.79	102.79	112.71
8	A	2021	Y01	CBH-CBF-CBD	-6.78	102.80	112.71
8	A	2022	Y01	CAS-CBF-CBH	-6.63	104.91	113.08
8	A	2008	Y01	CBH-CBF-CBD	-6.51	103.20	112.71
8	A	2026	Y01	CBH-CBF-CBD	-6.47	103.26	112.71
8	A	2025	Y01	CBH-CBF-CBD	-6.44	103.30	112.71
8	A	2020	Y01	CBH-CBF-CBD	-6.43	103.32	112.71
8	A	2007	Y01	CBH-CBF-CBD	-6.38	103.39	112.71
8	A	2016	Y01	CBH-CBF-CBD	-6.37	103.41	112.71
8	A	2015	Y01	CBH-CBF-CBD	-6.34	103.45	112.71
8	A	2011	Y01	CBH-CBF-CBD	-6.31	103.49	112.71
8	A	2003	Y01	CAS-CBF-CBH	-6.23	105.40	113.08
8	A	2013	Y01	CAD-CBH-CAZ	6.19	117.84	108.38
11	E	301	GSP	C5-C4-N3	-6.13	118.63	128.39
8	H	102	Y01	CBH-CBF-CBD	-6.12	103.78	112.71
8	A	2022	Y01	CBH-CBF-CBD	-6.10	103.80	112.71
8	A	2019	Y01	CBH-CBF-CBD	-6.06	103.85	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2014	Y01	CBH-CBF-CBD	-6.06	103.86	112.71
8	A	2023	Y01	CBH-CBF-CBD	-6.03	103.91	112.71
8	A	2008	Y01	CAS-CBF-CBH	-5.98	105.71	113.08
8	A	2030	Y01	CBH-CBF-CBD	-5.97	103.98	112.71
8	A	2002	Y01	CBH-CAZ-CAI	-5.91	114.30	122.93
8	A	2002	Y01	CBH-CBF-CBD	-5.83	104.19	112.71
8	A	2021	Y01	CBI-CBE-CBB	-5.83	110.50	119.50
8	A	2025	Y01	CAS-CBF-CBH	-5.80	105.93	113.08
8	A	2018	Y01	CBI-CBE-CBB	-5.76	110.60	119.50
8	A	2023	Y01	CAS-CBF-CBH	-5.75	106.00	113.08
8	A	2010	Y01	CBH-CAZ-CAI	-5.74	114.55	122.93
8	A	2030	Y01	CAS-CBF-CBH	-5.74	106.01	113.08
8	A	2024	Y01	CBH-CBF-CBD	-5.72	104.36	112.71
8	A	2004	Y01	CAD-CBH-CAZ	5.70	117.10	108.38
8	A	2024	Y01	CAS-CBF-CBH	-5.70	106.05	113.08
8	A	2027	Y01	CAS-CBF-CBH	-5.70	106.06	113.08
8	A	2005	Y01	CAK-CBD-CBG	5.69	118.99	110.93
8	A	2004	Y01	CBC-CAV-CAZ	5.68	119.84	111.45
8	A	2012	Y01	CAS-CBF-CBH	-5.64	106.13	113.08
8	A	2007	Y01	CAD-CBH-CAZ	5.64	117.00	108.38
8	A	2027	Y01	CBH-CAZ-CAI	-5.64	114.70	122.93
8	A	2020	Y01	CAS-CBF-CBH	-5.64	106.14	113.08
8	A	2020	Y01	CBH-CAZ-CAI	-5.63	114.71	122.93
8	H	102	Y01	CAD-CBH-CAZ	5.62	116.97	108.38
8	A	2019	Y01	CAS-CBF-CBH	-5.62	106.15	113.08
8	A	2026	Y01	CAS-CBF-CBH	-5.62	106.16	113.08
8	A	2016	Y01	CAS-CBF-CBH	-5.60	106.18	113.08
8	A	2008	Y01	CAK-CBD-CBF	-5.59	103.26	109.72
8	A	2010	Y01	CAS-CBF-CBH	-5.54	106.25	113.08
8	A	2017	Y01	CBH-CAZ-CAI	-5.54	114.83	122.93
8	A	2016	Y01	CBH-CAZ-CAI	-5.54	114.83	122.93
8	A	2023	Y01	CBH-CAZ-CAI	-5.53	114.86	122.93
8	A	2004	Y01	CBH-CBF-CBD	-5.46	104.73	112.71
10	A	2031	UDP	C4-N3-C2	-5.44	119.85	126.61
8	A	2002	Y01	CAS-CBF-CBH	-5.42	106.40	113.08
8	A	2013	Y01	CBF-CBH-CAZ	-5.40	101.74	109.65
8	A	2015	Y01	CBI-CBE-CBB	-5.38	111.19	119.50
8	A	2029	Y01	CBI-CBE-CBB	-5.36	111.22	119.50
8	A	2018	Y01	CBH-CAZ-CAI	-5.35	115.12	122.93
8	A	2017	Y01	CAS-CBF-CBH	-5.34	106.50	113.08
11	E	301	GSP	C1'-N9-C4	-5.29	110.85	126.49
8	A	2019	Y01	CBI-CBE-CBB	-5.26	111.37	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2014	Y01	CBI-CBE-CBB	-5.25	111.39	119.50
8	A	2027	Y01	CBH-CBF-CBD	-5.24	105.05	112.71
11	E	301	GSP	C1'-N9-C8	5.23	141.59	126.73
8	A	2015	Y01	CAS-CBF-CBH	-5.23	106.64	113.08
8	A	2009	Y01	CAS-CBF-CBH	-5.23	106.64	113.08
8	A	2003	Y01	CAD-CBH-CAZ	5.20	116.33	108.38
8	A	2026	Y01	CBI-CBE-CBB	-5.19	111.48	119.50
8	A	2029	Y01	CAS-CBF-CBH	-5.17	106.72	113.08
8	A	2005	Y01	CAK-CBD-CBF	-5.16	103.76	109.72
8	A	2025	Y01	CBH-CAZ-CAI	-5.14	115.43	122.93
8	A	2003	Y01	CBH-CBF-CBD	-5.11	105.25	112.71
8	A	2030	Y01	CAD-CBH-CAZ	5.10	116.17	108.38
8	A	2013	Y01	CBF-CBD-CBG	-5.09	102.44	109.09
8	A	2018	Y01	CAS-CBF-CBH	-5.08	106.82	113.08
8	A	2027	Y01	CAD-CBH-CAZ	5.07	116.13	108.38
8	A	2021	Y01	CAS-CBF-CBH	-5.07	106.84	113.08
8	A	2008	Y01	CAV-CAZ-CBH	-5.06	109.94	116.42
8	A	2002	Y01	CBI-CBE-CBB	-5.05	111.70	119.50
8	A	2005	Y01	CAD-CBH-CAZ	5.03	116.07	108.38
8	A	2027	Y01	CBI-CBE-CBB	-5.03	111.73	119.50
8	A	2009	Y01	CBH-CAZ-CAI	-5.02	115.59	122.93
8	A	2025	Y01	CBI-CBE-CBB	-5.02	111.75	119.50
8	A	2012	Y01	CAD-CBH-CAZ	5.01	116.03	108.38
8	A	2028	Y01	CAD-CBH-CAZ	4.99	116.01	108.38
8	A	2002	Y01	CAD-CBH-CAZ	4.98	116.00	108.38
8	A	2024	Y01	CBI-CBE-CBB	-4.97	111.82	119.50
8	A	2012	Y01	CBI-CBE-CBB	-4.97	111.83	119.50
8	A	2010	Y01	CAD-CBH-CAZ	4.97	115.97	108.38
8	A	2023	Y01	CAD-CBH-CAZ	4.96	115.97	108.38
8	A	2014	Y01	CAD-CBH-CAZ	4.96	115.96	108.38
8	A	2016	Y01	CAD-CBH-CAZ	4.94	115.93	108.38
11	E	301	GSP	C2-N3-C4	4.94	120.81	112.30
8	A	2015	Y01	CAD-CBH-CAZ	4.94	115.93	108.38
8	A	2017	Y01	CBI-CBE-CBB	-4.93	111.88	119.50
8	A	2011	Y01	CAD-CBH-CAZ	4.93	115.92	108.38
8	A	2020	Y01	CAD-CBH-CAZ	4.93	115.91	108.38
8	A	2022	Y01	CAD-CBH-CAZ	4.91	115.88	108.38
8	A	2021	Y01	CAD-CBH-CAZ	4.91	115.88	108.38
8	A	2015	Y01	CBH-CAZ-CAI	-4.91	115.77	122.93
8	A	2017	Y01	CAD-CBH-CAZ	4.91	115.88	108.38
8	A	2029	Y01	CBH-CAZ-CAI	-4.90	115.77	122.93
8	A	2008	Y01	CBD-CAK-CAI	-4.89	105.99	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2029	Y01	CAK-CBD-CBF	-4.89	104.07	109.72
8	A	2025	Y01	CAD-CBH-CAZ	4.88	115.84	108.38
8	A	2009	Y01	CAK-CBD-CBF	-4.88	104.09	109.72
8	A	2016	Y01	CBI-CBE-CBB	-4.87	111.97	119.50
8	A	2026	Y01	CAD-CBH-CAZ	4.85	115.79	108.38
8	A	2009	Y01	CAD-CBH-CAZ	4.84	115.78	108.38
8	A	2008	Y01	CAD-CBH-CAZ	4.84	115.77	108.38
8	A	2013	Y01	CBH-CBF-CBD	-4.83	105.65	112.71
8	A	2024	Y01	CAD-CBH-CAZ	4.81	115.73	108.38
8	A	2007	Y01	CAS-CBF-CBH	-4.81	107.16	113.08
8	A	2019	Y01	CAD-CBH-CAZ	4.78	115.69	108.38
8	A	2024	Y01	CBH-CAZ-CAI	-4.78	115.95	122.93
8	A	2029	Y01	CAD-CBH-CAZ	4.73	115.61	108.38
8	A	2026	Y01	CBH-CAZ-CAI	-4.73	116.02	122.93
8	A	2012	Y01	CBH-CAZ-CAI	-4.73	116.02	122.93
8	A	2018	Y01	CAD-CBH-CAZ	4.72	115.60	108.38
8	A	2010	Y01	CBI-CBE-CBB	-4.69	112.25	119.50
8	A	2030	Y01	CAV-CAZ-CBH	-4.67	110.45	116.42
8	A	2020	Y01	CAU-CBI-CBE	-4.66	109.73	116.60
8	A	2004	Y01	CBI-CBE-CBB	-4.66	112.30	119.50
8	A	2008	Y01	CBI-CBE-CBB	-4.66	112.30	119.50
8	A	2021	Y01	CBH-CAZ-CAI	-4.66	116.13	122.93
8	A	2014	Y01	CBH-CAZ-CAI	-4.64	116.16	122.93
8	A	2022	Y01	CBH-CAZ-CAI	-4.63	116.16	122.93
8	H	102	Y01	CBI-CBE-CBB	-4.63	112.34	119.50
8	A	2029	Y01	CAU-CBI-CBE	-4.60	109.82	116.60
8	A	2013	Y01	CBI-CBE-CBB	-4.60	112.39	119.50
8	A	2013	Y01	CAK-CBD-CBG	4.60	117.45	110.93
8	A	2020	Y01	CBI-CBE-CBB	-4.59	112.41	119.50
8	A	2014	Y01	CAS-CBF-CBH	-4.58	107.43	113.08
8	A	2009	Y01	CAU-CBI-CBE	-4.58	109.86	116.60
8	A	2016	Y01	CAU-CBI-CBE	-4.58	109.86	116.60
8	A	2005	Y01	CBD-CAK-CAI	-4.57	106.43	112.76
8	A	2005	Y01	CBI-CBE-CBB	-4.57	112.44	119.50
8	A	2028	Y01	CAS-CBF-CBH	-4.57	107.46	113.08
8	A	2005	Y01	CBH-CAZ-CAI	-4.56	116.27	122.93
11	E	301	GSP	PB-O3B-PG	-4.56	116.48	133.17
8	A	2017	Y01	CAU-CBI-CBE	-4.56	109.89	116.60
8	A	2004	Y01	CBF-CBD-CBG	-4.55	103.14	109.09
8	A	2005	Y01	CBI-CBG-CBD	-4.55	107.96	114.41
8	A	2015	Y01	CAU-CBI-CBE	-4.53	109.92	116.60
8	A	2009	Y01	CBI-CBE-CBB	-4.53	112.50	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2029	Y01	CAK-CBD-CBG	4.52	117.33	110.93
8	A	2005	Y01	CAV-CAZ-CBH	-4.52	110.64	116.42
8	A	2009	Y01	CAK-CBD-CBG	4.52	117.33	110.93
8	A	2026	Y01	CAU-CBI-CBE	-4.50	109.97	116.60
8	A	2012	Y01	CAV-CAZ-CBH	-4.48	110.69	116.42
8	A	2027	Y01	CAU-CBI-CBE	-4.47	110.02	116.60
8	A	2021	Y01	CAU-CBI-CBE	-4.47	110.02	116.60
8	A	2002	Y01	CAU-CBI-CBE	-4.46	110.03	116.60
8	A	2025	Y01	CAU-CBI-CBE	-4.45	110.04	116.60
8	A	2019	Y01	CBH-CAZ-CAI	-4.43	116.46	122.93
8	A	2024	Y01	CAU-CBI-CBE	-4.42	110.08	116.60
8	A	2003	Y01	CAV-CAZ-CBH	-4.42	110.76	116.42
8	A	2021	Y01	CBI-CBG-CBD	-4.42	108.14	114.41
8	A	2012	Y01	CAU-CBI-CBE	-4.42	110.09	116.60
8	A	2019	Y01	CAU-CBI-CBE	-4.41	110.11	116.60
8	A	2011	Y01	CBI-CBE-CBB	-4.40	112.70	119.50
8	A	2018	Y01	CAU-CBI-CBE	-4.39	110.13	116.60
8	A	2010	Y01	CAU-CBI-CBE	-4.39	110.13	116.60
8	A	2019	Y01	CAV-CAZ-CBH	-4.39	110.80	116.42
8	A	2014	Y01	CAU-CBI-CBE	-4.38	110.15	116.60
8	A	2003	Y01	CBH-CAZ-CAI	-4.36	116.56	122.93
8	A	2003	Y01	CAU-CBI-CBE	-4.36	110.17	116.60
8	A	2030	Y01	CAU-CBI-CBE	-4.36	110.17	116.60
8	A	2008	Y01	CAU-CBI-CBE	-4.36	110.18	116.60
8	A	2008	Y01	OAW-CAY-CAM	4.35	120.90	111.48
8	A	2029	Y01	CAS-CBF-CBD	4.35	117.84	111.78
8	A	2021	Y01	CAK-CBD-CBG	4.33	117.07	110.93
8	A	2011	Y01	CAS-CBF-CBH	-4.31	107.77	113.08
8	A	2022	Y01	CAV-CAZ-CBH	-4.31	110.90	116.42
8	A	2030	Y01	CBH-CAZ-CAI	-4.31	116.64	122.93
8	A	2022	Y01	CAU-CBI-CBE	-4.30	110.26	116.60
8	A	2004	Y01	CAK-CBD-CBG	4.29	117.01	110.93
8	A	2007	Y01	CAU-CBI-CBE	-4.29	110.28	116.60
8	A	2009	Y01	CAS-CBF-CBD	4.25	117.70	111.78
8	A	2011	Y01	CAU-CBI-CBE	-4.23	110.38	116.60
8	A	2014	Y01	CAK-CBD-CBG	4.22	116.91	110.93
8	A	2008	Y01	CAK-CBD-CBG	4.21	116.90	110.93
8	H	102	Y01	CBF-CBH-CAZ	-4.21	103.49	109.65
8	A	2005	Y01	CAS-CBF-CBH	-4.21	107.89	113.08
8	A	2005	Y01	CAU-CBI-CBE	-4.20	110.42	116.60
8	A	2028	Y01	CAU-CBI-CBE	-4.19	110.42	116.60
8	A	2004	Y01	CAR-CBC-CAV	4.18	116.79	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2014	Y01	CBI-CBG-CBD	-4.18	108.48	114.41
8	A	2015	Y01	CAK-CBD-CBG	4.18	116.85	110.93
8	A	2030	Y01	CBI-CBE-CBB	-4.17	113.06	119.50
8	A	2022	Y01	CAK-CBD-CBF	-4.15	104.93	109.72
8	A	2004	Y01	CAU-CBI-CBE	-4.14	110.50	116.60
8	A	2021	Y01	CAV-CAZ-CBH	-4.13	111.13	116.42
8	A	2014	Y01	CAV-CAZ-CBH	-4.13	111.14	116.42
8	A	2012	Y01	CAK-CBD-CBF	-4.12	104.96	109.72
8	A	2007	Y01	CBI-CBE-CBB	-4.11	113.14	119.50
8	A	2008	Y01	CBH-CAZ-CAI	-4.11	116.93	122.93
8	A	2026	Y01	CAV-CAZ-CBH	-4.07	111.21	116.42
8	A	2023	Y01	CAU-CBI-CBE	-4.06	110.61	116.60
8	A	2022	Y01	CBI-CBE-CBB	-4.06	113.23	119.50
8	A	2023	Y01	OAW-CAY-CAM	4.06	120.25	111.48
8	A	2012	Y01	OAW-CAY-CAM	4.05	120.23	111.48
8	A	2017	Y01	CAS-CBF-CBD	4.04	117.42	111.78
8	A	2025	Y01	OAW-CAY-CAM	4.04	120.22	111.48
8	A	2029	Y01	CAV-CAZ-CBH	-4.03	111.26	116.42
8	A	2017	Y01	OAW-CAY-CAM	4.02	120.17	111.48
8	A	2009	Y01	OAW-CAY-CAM	4.01	120.16	111.48
8	A	2030	Y01	CAK-CBD-CBG	4.01	116.60	110.93
8	A	2030	Y01	CAK-CBD-CBF	-4.00	105.09	109.72
8	A	2002	Y01	OAW-CAY-CAM	4.00	120.14	111.48
8	A	2014	Y01	OAW-CAY-CAM	3.99	120.10	111.48
8	A	2008	Y01	CAS-CBF-CBD	3.98	117.33	111.78
11	E	301	GSP	N9-C4-N3	3.98	133.91	125.95
8	A	2017	Y01	CAK-CBD-CBG	3.98	116.56	110.93
8	A	2015	Y01	CBI-CBG-CBD	-3.97	108.78	114.41
10	A	2031	UDP	N3-C2-N1	3.97	120.05	114.89
8	A	2021	Y01	CAK-CBD-CBF	-3.96	105.14	109.72
8	A	2011	Y01	OAW-CAY-CAM	3.96	120.05	111.48
8	A	2026	Y01	OAW-CAY-CAM	3.96	120.04	111.48
8	A	2019	Y01	OAW-CAY-CAM	3.96	120.04	111.48
8	H	102	Y01	CBF-CBD-CBG	-3.94	103.94	109.09
8	A	2003	Y01	OAW-CAY-CAM	3.94	120.00	111.48
8	A	2021	Y01	CAS-CBF-CBD	3.94	117.27	111.78
8	A	2015	Y01	OAW-CAY-CAM	3.92	119.97	111.48
8	A	2010	Y01	CAK-CBD-CBF	-3.92	105.19	109.72
8	A	2012	Y01	CAS-CBF-CBD	3.92	117.25	111.78
8	A	2027	Y01	OAW-CAY-CAM	3.92	119.96	111.48
8	A	2010	Y01	OAW-CAY-CAM	3.92	119.95	111.48
8	A	2015	Y01	CAV-CAZ-CBH	-3.91	111.42	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2004	Y01	OAW-CAY-CAM	3.91	119.93	111.48
8	H	102	Y01	CAU-CBI-CBE	-3.90	110.85	116.60
8	A	2029	Y01	OAW-CAY-CAM	3.90	119.91	111.48
8	A	2024	Y01	OAW-CAY-CAM	3.89	119.89	111.48
8	A	2009	Y01	CAV-CAZ-CBH	-3.88	111.45	116.42
8	A	2013	Y01	CAU-CBI-CBE	-3.87	110.90	116.60
8	A	2005	Y01	OAW-CAY-CAM	3.87	119.84	111.48
8	A	2018	Y01	CAS-CBF-CBD	3.86	117.17	111.78
8	A	2030	Y01	OAW-CAY-CAM	3.86	119.83	111.48
8	A	2028	Y01	OAW-CAY-CAM	3.85	119.81	111.48
8	A	2016	Y01	OAW-CAY-CAM	3.85	119.81	111.48
8	A	2007	Y01	OAW-CAY-CAM	3.84	119.80	111.48
8	A	2026	Y01	CAK-CBD-CBF	-3.84	105.28	109.72
8	H	102	Y01	CAK-CBD-CBG	3.84	116.37	110.93
8	H	102	Y01	OAW-CAY-CAM	3.84	119.78	111.48
8	A	2013	Y01	OAW-CAY-CAM	3.84	119.78	111.48
8	A	2024	Y01	CAV-CAZ-CBH	-3.83	111.51	116.42
8	A	2028	Y01	CBI-CBE-CBB	-3.83	113.58	119.50
8	A	2029	Y01	CBI-CBG-CBD	-3.82	109.00	114.41
8	A	2004	Y01	CAD-CBH-CAT	3.81	115.23	109.43
8	A	2014	Y01	CAK-CBD-CBF	-3.80	105.33	109.72
8	A	2004	Y01	CBF-CBH-CAZ	-3.80	104.10	109.65
8	H	102	Y01	CAD-CBH-CAT	3.79	115.19	109.43
8	A	2009	Y01	CBI-CBG-CBD	-3.78	109.05	114.41
8	A	2007	Y01	CAK-CBD-CBG	3.77	116.27	110.93
8	A	2022	Y01	OAW-CAY-CAM	3.76	119.61	111.48
8	A	2007	Y01	CAD-CBH-CAT	3.75	115.13	109.43
8	A	2030	Y01	CAU-CAS-CBF	3.74	119.50	113.14
8	A	2026	Y01	CAS-CBF-CBD	3.73	116.99	111.78
8	A	2029	Y01	CBD-CAK-CAI	-3.73	107.60	112.76
8	A	2017	Y01	CAK-CBD-CBF	-3.71	105.43	109.72
10	A	2031	UDP	C5-C4-N3	3.71	119.99	114.80
8	A	2019	Y01	CAK-CBD-CBF	-3.71	105.44	109.72
8	A	2015	Y01	CAU-CAS-CBF	3.70	119.42	113.14
8	A	2013	Y01	CAD-CBH-CAT	3.68	115.04	109.43
8	A	2020	Y01	CAS-CBF-CBD	3.68	116.92	111.78
8	A	2010	Y01	CAS-CBF-CBD	3.68	116.91	111.78
8	A	2007	Y01	CBC-CAV-CAZ	3.67	116.88	111.45
8	A	2014	Y01	CAU-CAS-CBF	3.65	119.34	113.14
8	A	2020	Y01	OAW-CAY-CAM	3.63	119.34	111.48
8	A	2020	Y01	CAK-CBD-CBG	3.63	116.08	110.93
8	A	2030	Y01	CBD-CAK-CAI	-3.63	107.74	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2020	Y01	CAK-CBD-CBF	-3.62	105.53	109.72
8	A	2015	Y01	CAS-CBF-CBD	3.61	116.82	111.78
8	A	2018	Y01	OAW-CAY-CAM	3.60	119.28	111.48
8	A	2009	Y01	CBD-CAK-CAI	-3.60	107.77	112.76
8	A	2030	Y01	CBI-CBG-CBD	-3.59	109.32	114.41
8	A	2013	Y01	CAD-CBH-CBF	3.58	115.68	111.66
8	A	2026	Y01	CAK-CBD-CBG	3.58	116.00	110.93
8	A	2021	Y01	OAW-CAY-CAM	3.58	119.22	111.48
8	A	2019	Y01	CAS-CBF-CBD	3.56	116.74	111.78
8	A	2025	Y01	CAV-CAZ-CBH	-3.52	111.92	116.42
8	A	2025	Y01	CAK-CBD-CBF	-3.52	105.65	109.72
8	A	2025	Y01	CAS-CBF-CBD	3.51	116.68	111.78
8	A	2012	Y01	CAK-CBD-CBG	3.51	115.90	110.93
8	A	2021	Y01	CBD-CAK-CAI	-3.51	107.90	112.76
8	A	2021	Y01	CAU-CAS-CBF	3.50	119.09	113.14
8	A	2015	Y01	CAK-CBD-CBF	-3.50	105.67	109.72
8	A	2014	Y01	CBD-CAK-CAI	-3.49	107.92	112.76
8	A	2013	Y01	CBC-CAV-CAZ	3.48	116.59	111.45
8	A	2016	Y01	CAK-CBD-CBG	3.46	115.83	110.93
8	A	2016	Y01	CAS-CBF-CBD	3.45	116.60	111.78
8	A	2008	Y01	CBI-CBG-CBD	-3.45	109.51	114.41
8	A	2026	Y01	CAU-CAS-CBF	3.44	118.98	113.14
8	A	2003	Y01	CAU-CAS-CBF	3.44	118.98	113.14
8	A	2004	Y01	CAS-CBF-CBH	-3.42	108.87	113.08
8	A	2029	Y01	CAU-CAS-CBF	3.40	118.91	113.14
8	A	2018	Y01	CAC-CBB-CBE	-3.39	107.79	112.88
8	A	2030	Y01	CAS-CBF-CBD	3.39	116.51	111.78
8	A	2020	Y01	CAD-CBH-CAT	3.39	114.59	109.43
8	A	2009	Y01	CAU-CAS-CBF	3.38	118.88	113.14
8	A	2011	Y01	CAD-CBH-CAT	3.38	114.57	109.43
11	E	301	GSP	C2-N1-C6	-3.37	118.99	125.11
8	A	2003	Y01	CBI-CBE-CBB	-3.35	114.32	119.50
8	A	2024	Y01	CAU-CAS-CBF	3.35	118.83	113.14
8	A	2009	Y01	CAD-CBH-CAT	3.34	114.51	109.43
8	A	2005	Y01	CAU-CAS-CBF	3.33	118.80	113.14
8	A	2018	Y01	CAK-CBD-CBF	-3.33	105.87	109.72
8	A	2029	Y01	CAD-CBH-CAT	3.32	114.49	109.43
8	A	2014	Y01	CAD-CBH-CAT	3.32	114.48	109.43
8	A	2020	Y01	CAV-CAZ-CBH	-3.32	112.17	116.42
8	A	2019	Y01	CAU-CAS-CBF	3.32	118.78	113.14
8	A	2007	Y01	CAR-CBC-CAV	3.32	115.58	110.97
8	A	2019	Y01	CAK-CBD-CBG	3.31	115.62	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2022	Y01	CAS-CBF-CBD	3.31	116.39	111.78
8	A	2005	Y01	CAD-CBH-CAT	3.30	114.45	109.43
8	A	2019	Y01	CBI-CBG-CBD	-3.29	109.75	114.41
8	A	2003	Y01	CAK-CBD-CBF	-3.28	105.93	109.72
8	H	102	Y01	CAS-CBF-CBH	-3.27	109.05	113.08
8	A	2026	Y01	CBI-CBG-CBD	-3.27	109.78	114.41
8	A	2028	Y01	CAD-CBH-CAT	3.26	114.39	109.43
8	A	2010	Y01	CAK-CBD-CBG	3.25	115.54	110.93
8	A	2018	Y01	CAD-CBH-CAT	3.25	114.38	109.43
8	A	2008	Y01	CAU-CAS-CBF	3.25	118.66	113.14
8	A	2013	Y01	CAR-CBC-CAV	3.24	115.48	110.97
8	A	2023	Y01	CAD-CBH-CAT	3.23	114.34	109.43
8	A	2008	Y01	CAT-CAR-CBC	3.21	115.58	110.33
8	A	2019	Y01	CBD-CAK-CAI	-3.21	108.31	112.76
8	A	2015	Y01	CAD-CBH-CAT	3.20	114.31	109.43
8	A	2016	Y01	CAD-CBH-CAT	3.20	114.30	109.43
8	A	2017	Y01	CAD-CBH-CAT	3.20	114.29	109.43
8	A	2008	Y01	CAR-CBC-CAV	3.18	115.40	110.97
8	A	2017	Y01	CAV-CAZ-CBH	-3.17	112.36	116.42
8	A	2014	Y01	CAS-CBF-CBD	3.16	116.19	111.78
8	A	2026	Y01	CAD-CBH-CAT	3.15	114.23	109.43
8	A	2011	Y01	CAK-CBD-CBG	3.15	115.39	110.93
8	A	2016	Y01	CAV-CAZ-CBH	-3.15	112.39	116.42
8	A	2010	Y01	CAD-CBH-CAT	3.15	114.22	109.43
8	A	2025	Y01	CAD-CBH-CAT	3.14	114.21	109.43
8	A	2008	Y01	CAD-CBH-CAT	3.13	114.19	109.43
8	A	2012	Y01	CAD-CBH-CAT	3.13	114.19	109.43
8	A	2005	Y01	CAS-CBF-CBD	3.13	116.14	111.78
8	A	2027	Y01	CAD-CBH-CAT	3.13	114.19	109.43
8	A	2019	Y01	CAD-CBH-CAT	3.11	114.17	109.43
8	A	2018	Y01	CAK-CBD-CBG	3.11	115.33	110.93
8	A	2002	Y01	CAD-CBH-CAT	3.10	114.15	109.43
8	A	2021	Y01	CAD-CBH-CAT	3.10	114.14	109.43
8	A	2022	Y01	CAD-CBH-CAT	3.10	114.14	109.43
8	A	2024	Y01	CAD-CBH-CAT	3.10	114.14	109.43
8	A	2024	Y01	CAS-CBF-CBD	3.10	116.10	111.78
8	A	2026	Y01	CBD-CAK-CAI	-3.10	108.47	112.76
8	A	2016	Y01	CAK-CBD-CBF	-3.09	106.15	109.72
8	A	2018	Y01	CBI-CBG-CBD	-3.09	110.03	114.41
10	A	2031	UDP	O4-C4-C5	-3.09	119.84	125.16
8	A	2012	Y01	CBD-CAK-CAI	-3.07	108.51	112.76
8	A	2025	Y01	CAK-CBD-CBG	3.07	115.28	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2023	Y01	CAV-CAZ-CBH	-3.07	112.50	116.42
8	A	2003	Y01	CAK-CBD-CBG	3.06	115.27	110.93
8	A	2007	Y01	CBI-CBG-CBD	-3.03	110.11	114.41
8	A	2017	Y01	CBI-CBG-CBD	-3.03	110.11	114.41
8	A	2024	Y01	CAK-CBD-CBG	3.03	115.22	110.93
8	A	2018	Y01	CAV-CAZ-CBH	-3.03	112.55	116.42
8	A	2004	Y01	CBI-CBG-CBD	-3.02	110.13	114.41
8	A	2004	Y01	CAD-CBH-CBF	3.02	115.05	111.66
8	A	2011	Y01	CBF-CBH-CAZ	-3.01	105.24	109.65
8	A	2012	Y01	CBI-CBG-CBD	-3.01	110.13	114.41
8	A	2022	Y01	CAK-CBD-CBG	3.00	115.19	110.93
8	A	2023	Y01	CBI-CBE-CBB	-3.00	114.86	119.50
8	A	2030	Y01	CAD-CBH-CAT	3.00	114.00	109.43
8	A	2012	Y01	CAU-CAS-CBF	2.99	118.22	113.14
8	A	2016	Y01	CBI-CBG-CBD	-2.99	110.17	114.41
8	A	2017	Y01	CAU-CAS-CBF	2.97	118.19	113.14
8	A	2027	Y01	CBF-CBD-CBG	-2.97	105.21	109.09
8	A	2028	Y01	CAK-CBD-CBG	2.96	115.13	110.93
8	A	2016	Y01	CAU-CAS-CBF	2.96	118.17	113.14
8	A	2015	Y01	CBD-CAK-CAI	-2.95	108.67	112.76
8	A	2028	Y01	CBF-CBH-CAZ	-2.95	105.34	109.65
8	A	2024	Y01	CBI-CBG-CBD	-2.94	110.24	114.41
8	A	2003	Y01	CAS-CBF-CBD	2.92	115.85	111.78
8	A	2022	Y01	CBD-CAK-CAI	-2.90	108.74	112.76
8	A	2028	Y01	CAS-CBF-CBD	2.88	115.80	111.78
8	A	2014	Y01	CBF-CBD-CBG	-2.88	105.33	109.09
8	H	102	Y01	CAD-CBH-CBF	2.87	114.88	111.66
8	A	2010	Y01	CAV-CAZ-CBH	-2.86	112.76	116.42
8	A	2007	Y01	CBF-CBH-CAZ	-2.85	105.48	109.65
8	A	2003	Y01	CBI-CBG-CBD	-2.84	110.38	114.41
8	A	2012	Y01	CAT-CAR-CBC	2.84	114.96	110.33
8	H	102	Y01	CBI-CBG-CBD	-2.83	110.40	114.41
11	E	301	GSP	C5-C6-N1	2.83	120.45	113.25
8	A	2003	Y01	CBD-CAK-CAI	-2.83	108.85	112.76
8	A	2020	Y01	CAU-CAS-CBF	2.82	117.93	113.14
8	A	2007	Y01	CBF-CBD-CBG	-2.82	105.41	109.09
8	A	2011	Y01	CBC-CAV-CAZ	2.81	115.61	111.45
8	A	2028	Y01	CAT-CBH-CAZ	2.81	113.58	108.74
8	A	2002	Y01	CAS-CBF-CBD	2.79	115.67	111.78
8	A	2025	Y01	CAU-CAS-CBF	2.78	117.86	113.14
8	A	2023	Y01	CAS-CBF-CBD	2.77	115.65	111.78
8	A	2005	Y01	CBF-CBD-CBG	-2.77	105.47	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2024	Y01	CAK-CBD-CBF	-2.73	106.57	109.72
8	A	2020	Y01	CBI-CBG-CBD	-2.72	110.55	114.41
8	A	2011	Y01	CAT-CBH-CAZ	2.67	113.35	108.74
8	A	2018	Y01	CAU-CAS-CBF	2.66	117.65	113.14
8	A	2027	Y01	CAV-CAZ-CBH	-2.65	113.03	116.42
8	A	2027	Y01	CAC-CBB-CBE	-2.64	108.92	112.88
8	A	2002	Y01	CAK-CBD-CBG	2.61	114.63	110.93
8	A	2013	Y01	CBI-CBG-CBD	-2.61	110.71	114.41
8	A	2021	Y01	CBG-CBI-CBE	2.60	103.08	100.10
8	A	2007	Y01	CAD-CBH-CBF	2.59	114.57	111.66
8	A	2022	Y01	CAU-CAS-CBF	2.59	117.54	113.14
11	E	301	GSP	O6-C6-C5	-2.57	119.75	126.53
8	A	2023	Y01	CAK-CBD-CBF	-2.56	106.77	109.72
8	A	2002	Y01	CAV-CAZ-CBH	-2.53	113.18	116.42
8	A	2003	Y01	CAD-CBH-CAT	2.50	113.23	109.43
8	A	2025	Y01	CBI-CBG-CBD	-2.50	110.87	114.41
8	A	2010	Y01	CAU-CAS-CBF	2.48	117.36	113.14
8	A	2022	Y01	CBI-CBG-CBD	-2.48	110.89	114.41
8	A	2028	Y01	CAK-CBD-CBF	-2.47	106.86	109.72
8	A	2015	Y01	CBF-CBD-CBG	-2.45	105.89	109.09
8	A	2002	Y01	CAC-CBB-CBE	-2.44	109.22	112.88
8	A	2013	Y01	CAS-CBF-CBH	-2.43	110.09	113.08
11	E	301	GSP	N9-C8-N7	-2.43	108.90	113.40
8	A	2004	Y01	CAP-CBE-CBB	-2.42	108.51	112.18
8	A	2003	Y01	CBF-CBD-CBG	-2.42	105.92	109.09
8	A	2008	Y01	CAP-CBE-CBB	-2.41	108.53	112.18
8	A	2024	Y01	CBF-CBD-CBG	-2.40	105.94	109.09
8	A	2025	Y01	CAC-CBB-CBE	-2.40	109.28	112.88
8	H	102	Y01	CAP-CBE-CBB	-2.40	108.54	112.18
8	A	2023	Y01	CAK-CBD-CBG	2.40	114.33	110.93
8	A	2027	Y01	CAK-CBD-CBG	2.39	114.32	110.93
8	A	2024	Y01	CAP-CBE-CBB	-2.39	108.56	112.18
8	A	2027	Y01	CAU-CAS-CBF	2.39	117.19	113.14
8	A	2026	Y01	CAC-CBB-CBE	-2.39	109.30	112.88
8	A	2003	Y01	CAP-CBE-CBB	-2.38	108.57	112.18
8	H	102	Y01	CAV-CAZ-CBH	-2.38	113.38	116.42
8	A	2029	Y01	CAC-CBB-CBE	-2.37	109.33	112.88
8	A	2018	Y01	CBD-CAK-CAI	-2.36	109.50	112.76
8	A	2030	Y01	CBF-CBD-CBG	-2.36	106.01	109.09
8	A	2019	Y01	CAC-CBB-CBE	-2.34	109.37	112.88
8	A	2025	Y01	CBD-CAK-CAI	-2.34	109.52	112.76
8	A	2011	Y01	CAS-CBF-CBD	2.33	115.03	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2015	Y01	CAC-CBB-CBE	-2.33	109.39	112.88
8	A	2005	Y01	CAP-CBE-CBB	-2.32	108.67	112.18
8	A	2009	Y01	CBG-CBI-CBE	2.30	102.74	100.10
8	A	2007	Y01	CAS-CBF-CBD	2.30	114.98	111.78
8	A	2017	Y01	CBD-CAK-CAI	-2.29	109.59	112.76
8	A	2008	Y01	CBC-CAV-CAZ	2.28	114.82	111.45
11	E	301	GSP	C5'-C4'-C3'	-2.28	107.00	115.21
8	A	2021	Y01	CAC-CBB-CBE	-2.27	109.47	112.88
8	A	2024	Y01	CAC-CBB-CBE	-2.27	109.47	112.88
8	A	2013	Y01	CAC-CBB-CBE	-2.24	109.52	112.88
8	A	2027	Y01	CBI-CBG-CBD	-2.24	111.23	114.41
8	A	2014	Y01	CAS-CAU-CBI	2.22	116.49	112.74
8	A	2012	Y01	CAP-CBE-CBB	-2.22	108.82	112.18
8	A	2024	Y01	CBD-CAK-CAI	-2.22	109.69	112.76
8	A	2002	Y01	CAU-CAS-CBF	2.22	116.90	113.14
8	A	2022	Y01	CAP-CBE-CBB	-2.21	108.83	112.18
8	A	2011	Y01	CBF-CBD-CBG	-2.20	106.21	109.09
8	A	2010	Y01	CAC-CBB-CBE	-2.20	109.58	112.88
8	A	2013	Y01	CAU-CBI-CBG	2.19	110.52	107.25
8	A	2012	Y01	CAC-CBB-CBE	-2.18	109.61	112.88
8	A	2011	Y01	CAD-CBH-CBF	2.18	114.10	111.66
8	A	2017	Y01	CBG-CBI-CBE	2.17	102.59	100.10
8	A	2014	Y01	CAC-CBB-CBE	-2.17	109.63	112.88
8	A	2010	Y01	CBI-CBG-CBD	-2.17	111.34	114.41
8	A	2002	Y01	CAD-CBH-CBF	2.16	114.08	111.66
8	A	2027	Y01	CAS-CBF-CBD	2.15	114.78	111.78
8	A	2003	Y01	CAS-CAU-CBI	2.14	116.35	112.74
8	A	2002	Y01	CAT-CBH-CAZ	2.13	112.42	108.74
10	A	2031	UDP	O2-C2-N1	-2.13	120.03	122.80
8	A	2030	Y01	CAS-CAU-CBI	2.12	116.33	112.74
8	A	2009	Y01	CAP-CBE-CBB	-2.12	108.96	112.18
8	A	2014	Y01	CAP-CBE-CBB	-2.11	108.98	112.18
8	A	2021	Y01	CAP-CBE-CBB	-2.10	109.00	112.18
8	A	2013	Y01	CBC-OAW-CAY	-2.10	112.77	117.80
8	A	2020	Y01	CAD-CBH-CBF	2.09	114.00	111.66
8	A	2027	Y01	CAT-CBH-CAZ	2.08	112.33	108.74
8	A	2007	Y01	CAP-CBE-CBB	-2.08	109.03	112.18
8	A	2003	Y01	CAD-CBH-CBF	2.07	113.99	111.66
8	A	2018	Y01	CAT-CBH-CAZ	2.07	112.31	108.74
8	A	2030	Y01	CAP-CBE-CBB	-2.06	109.07	112.18
8	A	2019	Y01	CAP-CBE-CBB	-2.05	109.08	112.18
8	A	2023	Y01	CAD-CBH-CBF	2.05	113.96	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2008	Y01	CBG-CBI-CBE	2.04	102.44	100.10
8	A	2029	Y01	CBG-CBI-CBE	2.03	102.42	100.10
8	A	2007	Y01	CAV-CAZ-CBH	-2.02	113.83	116.42
8	A	2002	Y01	CAK-CBD-CBF	-2.02	107.38	109.72
8	A	2016	Y01	CBG-CBI-CBE	2.02	102.41	100.10
8	A	2002	Y01	CBI-CBG-CBD	-2.02	111.55	114.41
8	A	2016	Y01	CAP-CBE-CBB	-2.01	109.14	112.18
8	A	2023	Y01	CAT-CBH-CAZ	2.01	112.21	108.74
8	A	2010	Y01	CAD-CBH-CBF	2.00	113.91	111.66
8	A	2014	Y01	CAD-CBH-CBF	2.00	113.91	111.66
8	A	2016	Y01	CAD-CBH-CBF	2.00	113.91	111.66
8	A	2008	Y01	CAC-CBB-CBE	-2.00	109.88	112.88

There are no chirality outliers.

All (360) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2002	Y01	CAC-CBB-CBE-CBI
8	A	2003	Y01	CAM-CAY-OAW-CBC
8	A	2007	Y01	OAG-CAY-OAW-CBC
8	A	2007	Y01	CAM-CAY-OAW-CBC
8	A	2008	Y01	OAG-CAY-OAW-CBC
8	A	2008	Y01	CAM-CAY-OAW-CBC
8	A	2012	Y01	OAG-CAY-OAW-CBC
8	A	2012	Y01	CAM-CAY-OAW-CBC
8	A	2013	Y01	CAM-CAY-OAW-CBC
8	A	2015	Y01	CAO-CBB-CBE-CAP
8	A	2015	Y01	CAO-CBB-CBE-CBI
8	A	2015	Y01	CAC-CBB-CBE-CBI
8	A	2015	Y01	CAV-CBC-OAW-CAY
8	A	2015	Y01	CAM-CAY-OAW-CBC
8	A	2016	Y01	CAM-CAY-OAW-CBC
8	A	2017	Y01	CAM-CAY-OAW-CBC
8	A	2019	Y01	CAC-CBB-CBE-CBI
8	A	2020	Y01	CAV-CBC-OAW-CAY
8	A	2021	Y01	CAR-CBC-OAW-CAY
8	A	2024	Y01	CAV-CBC-OAW-CAY
8	A	2024	Y01	OAG-CAY-OAW-CBC
8	A	2024	Y01	CAM-CAY-OAW-CBC
8	A	2025	Y01	CAC-CBB-CBE-CBI
8	A	2026	Y01	CAC-CBB-CBE-CBI
8	A	2027	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
8	A	2030	Y01	OAG-CAY-OAW-CBC
8	A	2030	Y01	CAM-CAY-OAW-CBC
8	H	102	Y01	OAG-CAY-OAW-CBC
8	H	102	Y01	CAM-CAY-OAW-CBC
9	A	2006	3PE	C1-O11-P-O12
9	A	2006	3PE	C1-O11-P-O13
9	A	2006	3PE	C1-O11-P-O14
9	A	2006	3PE	O13-C11-C12-N
9	A	2006	3PE	C22-C21-O21-C2
10	A	2031	UDP	C5'-O5'-PA-O1A
10	A	2031	UDP	C5'-O5'-PA-O3A
12	H	101	A1CHR	O-C60-C61-C62
12	H	101	A1CHR	C69-C70-C71-C72
8	A	2025	Y01	CAO-CAJ-CAN-CBA
8	A	2014	Y01	CAV-CBC-OAW-CAY
8	A	2022	Y01	CAV-CBC-OAW-CAY
8	A	2026	Y01	CAV-CBC-OAW-CAY
8	A	2002	Y01	CAC-CBB-CBE-CAP
8	A	2015	Y01	CAC-CBB-CBE-CAP
8	A	2025	Y01	CAC-CBB-CBE-CAP
8	A	2026	Y01	CAC-CBB-CBE-CAP
8	A	2027	Y01	CAC-CBB-CBE-CAP
8	A	2018	Y01	CAC-CBB-CBE-CBI
8	A	2025	Y01	CAO-CBB-CBE-CBI
8	A	2026	Y01	CAO-CBB-CBE-CBI
8	A	2027	Y01	CAO-CBB-CBE-CBI
8	A	2013	Y01	OAG-CAY-OAW-CBC
8	A	2015	Y01	OAG-CAY-OAW-CBC
8	A	2016	Y01	OAG-CAY-OAW-CBC
8	A	2017	Y01	OAG-CAY-OAW-CBC
9	A	2006	3PE	O22-C21-O21-C2
8	A	2013	Y01	CAJ-CAO-CBB-CAC
8	A	2021	Y01	CAJ-CAO-CBB-CAC
8	A	2019	Y01	CAC-CBB-CBE-CAP
8	A	2023	Y01	CAO-CBB-CBE-CAP
8	A	2025	Y01	CAO-CBB-CBE-CAP
8	A	2026	Y01	CAO-CBB-CBE-CAP
8	A	2027	Y01	CAO-CBB-CBE-CAP
8	A	2002	Y01	CAO-CBB-CBE-CBI
8	A	2018	Y01	CAO-CBB-CBE-CBI
8	A	2019	Y01	CAO-CBB-CBE-CBI
8	A	2003	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
8	A	2009	Y01	CAJ-CAO-CBB-CAC
8	A	2012	Y01	CAJ-CAO-CBB-CBE
8	A	2015	Y01	CAJ-CAO-CBB-CBE
8	A	2017	Y01	CAJ-CAO-CBB-CBE
11	E	301	GSP	C3'-C4'-C5'-O5'
8	A	2003	Y01	CAJ-CAO-CBB-CAC
8	A	2011	Y01	CAJ-CAO-CBB-CAC
8	A	2017	Y01	CAJ-CAO-CBB-CAC
8	A	2018	Y01	CAJ-CAO-CBB-CAC
8	A	2022	Y01	CAJ-CAO-CBB-CAC
8	A	2027	Y01	CAJ-CAO-CBB-CAC
8	A	2003	Y01	CAJ-CAO-CBB-CBE
8	A	2005	Y01	CAJ-CAO-CBB-CBE
8	A	2008	Y01	CAJ-CAO-CBB-CBE
8	A	2009	Y01	CAJ-CAO-CBB-CBE
8	A	2011	Y01	CAJ-CAO-CBB-CBE
8	A	2013	Y01	CAJ-CAO-CBB-CBE
8	A	2016	Y01	CAJ-CAO-CBB-CBE
8	A	2018	Y01	CAJ-CAO-CBB-CBE
8	A	2022	Y01	CAJ-CAO-CBB-CBE
8	A	2027	Y01	CAJ-CAO-CBB-CBE
8	A	2030	Y01	CAJ-CAO-CBB-CBE
8	A	2005	Y01	CAJ-CAO-CBB-CAC
8	A	2008	Y01	CAJ-CAO-CBB-CAC
8	A	2015	Y01	CAJ-CAO-CBB-CAC
8	A	2002	Y01	CAJ-CAO-CBB-CBE
8	A	2020	Y01	CAJ-CAO-CBB-CBE
8	A	2026	Y01	CAJ-CAO-CBB-CBE
8	A	2007	Y01	CAJ-CAO-CBB-CAC
8	A	2016	Y01	CAJ-CAO-CBB-CAC
8	A	2019	Y01	CAO-CBB-CBE-CAP
8	A	2007	Y01	CAJ-CAO-CBB-CBE
8	A	2025	Y01	CAJ-CAO-CBB-CBE
8	H	102	Y01	CAJ-CAO-CBB-CBE
8	A	2020	Y01	CAM-CAY-OAW-CBC
8	A	2002	Y01	CAJ-CAO-CBB-CAC
8	A	2012	Y01	CAJ-CAO-CBB-CAC
8	A	2021	Y01	CAN-CAJ-CAO-CBB
8	A	2030	Y01	CAN-CAJ-CAO-CBB
8	A	2021	Y01	CAJ-CAO-CBB-CBE
8	A	2024	Y01	CAJ-CAO-CBB-CBE
8	A	2024	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
8	A	2027	Y01	CAR-CBC-OAW-CAY
8	A	2021	Y01	CAO-CAJ-CAN-CBA
8	A	2029	Y01	CAM-CAY-OAW-CBC
8	A	2002	Y01	CAO-CBB-CBE-CAP
8	A	2010	Y01	CAO-CAJ-CAN-CBA
8	A	2027	Y01	CAN-CAJ-CAO-CBB
8	A	2011	Y01	CAN-CAJ-CAO-CBB
8	A	2023	Y01	CAN-CAJ-CAO-CBB
8	H	102	Y01	CAN-CAJ-CAO-CBB
8	A	2014	Y01	CAR-CBC-OAW-CAY
8	A	2002	Y01	CAN-CAJ-CAO-CBB
8	A	2007	Y01	CAO-CAJ-CAN-CBA
8	A	2013	Y01	CAO-CAJ-CAN-CBA
8	A	2024	Y01	CAN-CAJ-CAO-CBB
8	A	2013	Y01	CAV-CBC-OAW-CAY
8	H	102	Y01	CAJ-CAO-CBB-CAC
8	A	2004	Y01	CAO-CAJ-CAN-CBA
8	A	2019	Y01	CAN-CAJ-CAO-CBB
8	A	2027	Y01	CAV-CBC-OAW-CAY
8	A	2005	Y01	CAO-CAJ-CAN-CBA
8	A	2030	Y01	CAJ-CAO-CBB-CAC
8	A	2020	Y01	OAG-CAY-OAW-CBC
8	A	2029	Y01	OAG-CAY-OAW-CBC
8	A	2018	Y01	CAV-CBC-OAW-CAY
8	A	2013	Y01	CAN-CAJ-CAO-CBB
8	A	2015	Y01	CAO-CAJ-CAN-CBA
8	A	2022	Y01	CAN-CAJ-CAO-CBB
8	A	2002	Y01	CAO-CAJ-CAN-CBA
8	A	2012	Y01	CAN-CAJ-CAO-CBB
8	A	2020	Y01	CAJ-CAO-CBB-CAC
8	A	2026	Y01	CAJ-CAO-CBB-CAC
8	A	2009	Y01	CAN-CAJ-CAO-CBB
8	A	2008	Y01	CAN-CAJ-CAO-CBB
8	A	2003	Y01	CAJ-CAN-CBA-CAB
8	A	2021	Y01	CAJ-CAN-CBA-CAB
8	A	2019	Y01	CAJ-CAO-CBB-CBE
8	A	2026	Y01	CAO-CAJ-CAN-CBA
8	A	2007	Y01	CAJ-CAN-CBA-CAB
8	A	2019	Y01	CAJ-CAN-CBA-CAA
8	A	2022	Y01	CAJ-CAN-CBA-CAA
8	A	2023	Y01	CAJ-CAN-CBA-CAA
8	A	2025	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
8	A	2026	Y01	CAJ-CAN-CBA-CAB
8	A	2028	Y01	CAJ-CAN-CBA-CAB
8	A	2017	Y01	CAX-CAL-CAM-CAY
8	A	2004	Y01	CAJ-CAN-CBA-CAB
8	A	2005	Y01	CAJ-CAN-CBA-CAB
8	A	2007	Y01	CAJ-CAN-CBA-CAA
8	A	2008	Y01	CAJ-CAN-CBA-CAA
8	A	2010	Y01	CAJ-CAN-CBA-CAB
8	A	2012	Y01	CAJ-CAN-CBA-CAA
8	A	2013	Y01	CAJ-CAN-CBA-CAB
8	A	2016	Y01	CAJ-CAN-CBA-CAB
8	A	2021	Y01	CAJ-CAN-CBA-CAA
8	A	2025	Y01	CAJ-CAN-CBA-CAA
8	A	2030	Y01	CAJ-CAN-CBA-CAA
8	A	2025	Y01	CAJ-CAO-CBB-CAC
8	A	2018	Y01	CAR-CBC-OAW-CAY
8	A	2002	Y01	CAJ-CAN-CBA-CAA
8	A	2004	Y01	CAJ-CAN-CBA-CAA
8	A	2008	Y01	CAJ-CAN-CBA-CAB
8	A	2011	Y01	CAJ-CAN-CBA-CAA
8	A	2013	Y01	CAJ-CAN-CBA-CAA
8	A	2014	Y01	CAJ-CAN-CBA-CAA
8	A	2015	Y01	CAJ-CAN-CBA-CAA
8	A	2016	Y01	CAJ-CAN-CBA-CAA
8	A	2018	Y01	CAJ-CAN-CBA-CAB
8	A	2019	Y01	CAJ-CAN-CBA-CAB
8	A	2022	Y01	CAJ-CAN-CBA-CAB
8	A	2023	Y01	CAJ-CAN-CBA-CAB
8	A	2026	Y01	CAJ-CAN-CBA-CAA
8	A	2028	Y01	CAJ-CAN-CBA-CAA
8	A	2029	Y01	CAJ-CAN-CBA-CAA
8	A	2028	Y01	CAO-CAJ-CAN-CBA
8	A	2021	Y01	CAM-CAY-OAW-CBC
12	H	101	A1CHR	C68-C69-C70-C71
8	A	2003	Y01	CAJ-CAN-CBA-CAA
8	A	2009	Y01	CAJ-CAN-CBA-CAB
8	A	2018	Y01	CAJ-CAN-CBA-CAA
8	A	2020	Y01	CAJ-CAN-CBA-CAA
8	A	2020	Y01	CAJ-CAN-CBA-CAB
8	A	2027	Y01	CAJ-CAN-CBA-CAA
8	A	2018	Y01	CAC-CBB-CBE-CAP
8	A	2012	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
8	H	102	Y01	CAJ-CAN-CBA-CAA
8	A	2005	Y01	CAM-CAY-OAW-CBC
8	A	2027	Y01	CAO-CAJ-CAN-CBA
8	A	2021	Y01	OAG-CAY-OAW-CBC
8	A	2003	Y01	CAO-CAJ-CAN-CBA
8	A	2003	Y01	CAO-CBB-CBE-CAP
8	A	2017	Y01	CAJ-CAN-CBA-CAB
8	A	2027	Y01	CAJ-CAN-CBA-CAB
8	A	2030	Y01	CAJ-CAN-CBA-CAB
8	H	102	Y01	CAJ-CAN-CBA-CAB
8	A	2015	Y01	CAN-CAJ-CAO-CBB
8	A	2018	Y01	CAN-CAJ-CAO-CBB
8	A	2019	Y01	CAJ-CAO-CBB-CAC
8	A	2022	Y01	CAM-CAY-OAW-CBC
8	A	2002	Y01	CAJ-CAN-CBA-CAB
8	A	2010	Y01	CAJ-CAN-CBA-CAA
8	A	2015	Y01	CAJ-CAN-CBA-CAB
8	A	2024	Y01	CAJ-CAN-CBA-CAA
9	A	2006	3PE	C32-C33-C34-C35
8	A	2005	Y01	CAJ-CAN-CBA-CAA
8	A	2014	Y01	CAJ-CAN-CBA-CAB
8	A	2009	Y01	CAO-CAJ-CAN-CBA
11	E	301	GSP	C4'-C5'-O5'-PA
8	A	2017	Y01	CAO-CAJ-CAN-CBA
9	A	2006	3PE	C39-C3A-C3B-C3C
9	A	2006	3PE	C3A-C3B-C3C-C3D
9	A	2006	3PE	O11-C1-C2-C3
11	E	301	GSP	O4'-C4'-C5'-O5'
8	A	2016	Y01	CAO-CAJ-CAN-CBA
8	A	2018	Y01	CAO-CAJ-CAN-CBA
8	A	2012	Y01	CAO-CAJ-CAN-CBA
8	A	2005	Y01	OAG-CAY-OAW-CBC
9	A	2006	3PE	C1-C2-C3-O31
8	A	2026	Y01	CAM-CAY-OAW-CBC
8	A	2024	Y01	CAO-CAJ-CAN-CBA
8	A	2023	Y01	CAC-CBB-CBE-CAP
9	A	2006	3PE	C35-C36-C37-C38
8	A	2020	Y01	CAO-CAJ-CAN-CBA
8	A	2024	Y01	CAJ-CAN-CBA-CAB
8	A	2020	Y01	CAX-CAL-CAM-CAY
9	A	2006	3PE	O21-C2-C3-O31
12	H	101	A1CHR	C75-C69-C70-C71

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Mol	Chain	Res	Type	Atoms
11	E	301	GSP	PA-O3A-PB-O1B
9	A	2006	3PE	C2-C1-O11-P
8	A	2023	Y01	CAO-CAJ-CAN-CBA
8	A	2010	Y01	CAN-CAJ-CAO-CBB
8	A	2022	Y01	OAG-CAY-OAW-CBC
8	A	2014	Y01	CAO-CAJ-CAN-CBA
8	A	2022	Y01	CAO-CAJ-CAN-CBA
8	A	2007	Y01	CAN-CAJ-CAO-CBB
9	A	2006	3PE	C2D-C2E-C2F-C2G
8	A	2023	Y01	CAM-CAY-OAW-CBC
8	A	2018	Y01	CAO-CBB-CBE-CAP
9	A	2006	3PE	C33-C34-C35-C36
8	A	2011	Y01	CAJ-CAN-CBA-CAB
8	A	2025	Y01	CAN-CAJ-CAO-CBB
8	A	2029	Y01	CAJ-CAN-CBA-CAB
8	A	2009	Y01	CAJ-CAN-CBA-CAA
8	A	2017	Y01	CAJ-CAN-CBA-CAA
8	A	2009	Y01	CAM-CAY-OAW-CBC
8	A	2002	Y01	CAR-CBC-OAW-CAY
8	A	2026	Y01	OAG-CAY-OAW-CBC
8	A	2010	Y01	CAJ-CAO-CBB-CBE
8	A	2011	Y01	CAO-CAJ-CAN-CBA
8	A	2002	Y01	CAV-CBC-OAW-CAY
8	A	2020	Y01	CAN-CAJ-CAO-CBB
8	A	2023	Y01	OAG-CAY-OAW-CBC
8	A	2023	Y01	CAC-CBB-CBE-CBI
8	A	2019	Y01	CAO-CAJ-CAN-CBA
8	A	2003	Y01	CAV-CBC-OAW-CAY
8	A	2009	Y01	OAG-CAY-OAW-CBC
9	A	2006	3PE	O11-C1-C2-O21
8	A	2025	Y01	CAM-CAY-OAW-CBC
8	A	2029	Y01	CAC-CBB-CBE-CBI
8	A	2003	Y01	CAN-CAJ-CAO-CBB
10	A	2031	UDP	C5'-O5'-PA-O2A
8	A	2004	Y01	CAN-CAJ-CAO-CBB
8	A	2008	Y01	CAO-CAJ-CAN-CBA
8	A	2017	Y01	CAN-CAJ-CAO-CBB
8	A	2023	Y01	CAO-CBB-CBE-CBI
8	A	2024	Y01	CAC-CBB-CBE-CBI
8	A	2013	Y01	CAR-CBC-OAW-CAY
8	A	2025	Y01	OAG-CAY-OAW-CBC
8	A	2019	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
8	A	2027	Y01	CAM-CAY-OAW-CBC
11	E	301	GSP	PB-O3A-PA-O2A
8	A	2019	Y01	OAG-CAY-OAW-CBC
8	A	2027	Y01	OAG-CAY-OAW-CBC
8	A	2003	Y01	CAR-CBC-OAW-CAY
8	A	2026	Y01	CAR-CBC-OAW-CAY
8	A	2011	Y01	OAG-CAY-OAW-CBC
8	H	102	Y01	CAO-CAJ-CAN-CBA
8	A	2014	Y01	OAG-CAY-OAW-CBC
9	A	2006	3PE	C27-C28-C29-C2A
8	A	2014	Y01	CAM-CAL-CAX-OAH
8	A	2019	Y01	CAM-CAL-CAX-OAH
8	A	2030	Y01	CAM-CAL-CAX-OAF
8	A	2019	Y01	CAM-CAL-CAX-OAF
8	A	2030	Y01	CAM-CAL-CAX-OAH
8	A	2023	Y01	CAJ-CAO-CBB-CAC
8	A	2010	Y01	CAV-CBC-OAW-CAY
8	A	2026	Y01	CAM-CAL-CAX-OAF
8	A	2015	Y01	CAM-CAL-CAX-OAH
8	A	2002	Y01	OAG-CAY-OAW-CBC
8	A	2003	Y01	CAM-CAL-CAX-OAF
8	A	2024	Y01	CAM-CAL-CAX-OAF
8	A	2011	Y01	CAM-CAY-OAW-CBC
8	A	2011	Y01	CAM-CAL-CAX-OAF
8	A	2026	Y01	CAM-CAL-CAX-OAH
8	A	2010	Y01	CAC-CBB-CBE-CBI
8	A	2015	Y01	CAM-CAL-CAX-OAF
8	A	2003	Y01	CAM-CAL-CAX-OAH
8	A	2021	Y01	CAM-CAL-CAX-OAF
8	A	2024	Y01	CAM-CAL-CAX-OAH
12	H	101	A1CHR	C67-C68-C69-C70
8	A	2021	Y01	CAM-CAL-CAX-OAH
8	A	2014	Y01	CAM-CAY-OAW-CBC
9	A	2006	3PE	C25-C26-C27-C28
8	A	2011	Y01	CAM-CAL-CAX-OAH
8	A	2002	Y01	CAM-CAY-OAW-CBC
8	A	2014	Y01	CAM-CAL-CAX-OAF
8	A	2022	Y01	CAM-CAL-CAX-OAH
8	H	102	Y01	CAM-CAL-CAX-OAH
8	A	2018	Y01	CAM-CAL-CAX-OAH
8	A	2018	Y01	CAM-CAL-CAX-OAF
8	A	2013	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
8	A	2021	Y01	CAC-CBB-CBE-CBI
8	A	2027	Y01	CAM-CAL-CAX-OAF
8	A	2016	Y01	CAM-CAL-CAX-OAH
8	A	2027	Y01	CAM-CAL-CAX-OAH
8	A	2014	Y01	CAC-CBB-CBE-CBI
8	A	2004	Y01	CAM-CAL-CAX-OAH
8	A	2029	Y01	CAM-CAL-CAX-OAH
8	A	2002	Y01	CAM-CAL-CAX-OAH
8	A	2022	Y01	CAM-CAL-CAX-OAF
8	H	102	Y01	CAM-CAL-CAX-OAF
8	A	2016	Y01	CAM-CAL-CAX-OAF
8	A	2002	Y01	CAM-CAL-CAX-OAF
8	A	2008	Y01	CAM-CAL-CAX-OAH
8	A	2004	Y01	CAM-CAL-CAX-OAF
8	A	2008	Y01	CAM-CAL-CAX-OAF
8	A	2029	Y01	CAM-CAL-CAX-OAF
8	A	2010	Y01	CAR-CBC-OAW-CAY
8	A	2028	Y01	CAV-CBC-OAW-CAY
8	A	2013	Y01	CAM-CAL-CAX-OAF
8	A	2019	Y01	CAL-CAM-CAY-OAW
8	A	2028	Y01	CAR-CBC-OAW-CAY
8	A	2023	Y01	CAM-CAL-CAX-OAH
8	A	2028	Y01	CAL-CAM-CAY-OAW
11	E	301	GSP	PB-O3A-PA-O1A
8	A	2014	Y01	CAL-CAM-CAY-OAW
8	A	2009	Y01	CAL-CAM-CAY-OAW
9	A	2006	3PE	C3B-C3C-C3D-C3E
9	A	2006	3PE	C2C-C2D-C2E-C2F
8	A	2023	Y01	CAM-CAL-CAX-OAF
8	A	2018	Y01	CAL-CAM-CAY-OAW
8	A	2029	Y01	CAO-CAJ-CAN-CBA
12	H	101	A1CHR	C67-C68-C69-C75
8	A	2019	Y01	CAL-CAM-CAY-OAG
8	A	2014	Y01	CAL-CAM-CAY-OAG
8	A	2028	Y01	CAL-CAM-CAY-OAG
8	A	2012	Y01	CAL-CAM-CAY-OAW
8	A	2029	Y01	CAN-CAJ-CAO-CBB
8	A	2018	Y01	CAL-CAM-CAY-OAG
8	A	2022	Y01	CAL-CAM-CAY-OAW
8	A	2009	Y01	CAL-CAM-CAY-OAG
8	A	2023	Y01	CAL-CAM-CAY-OAW

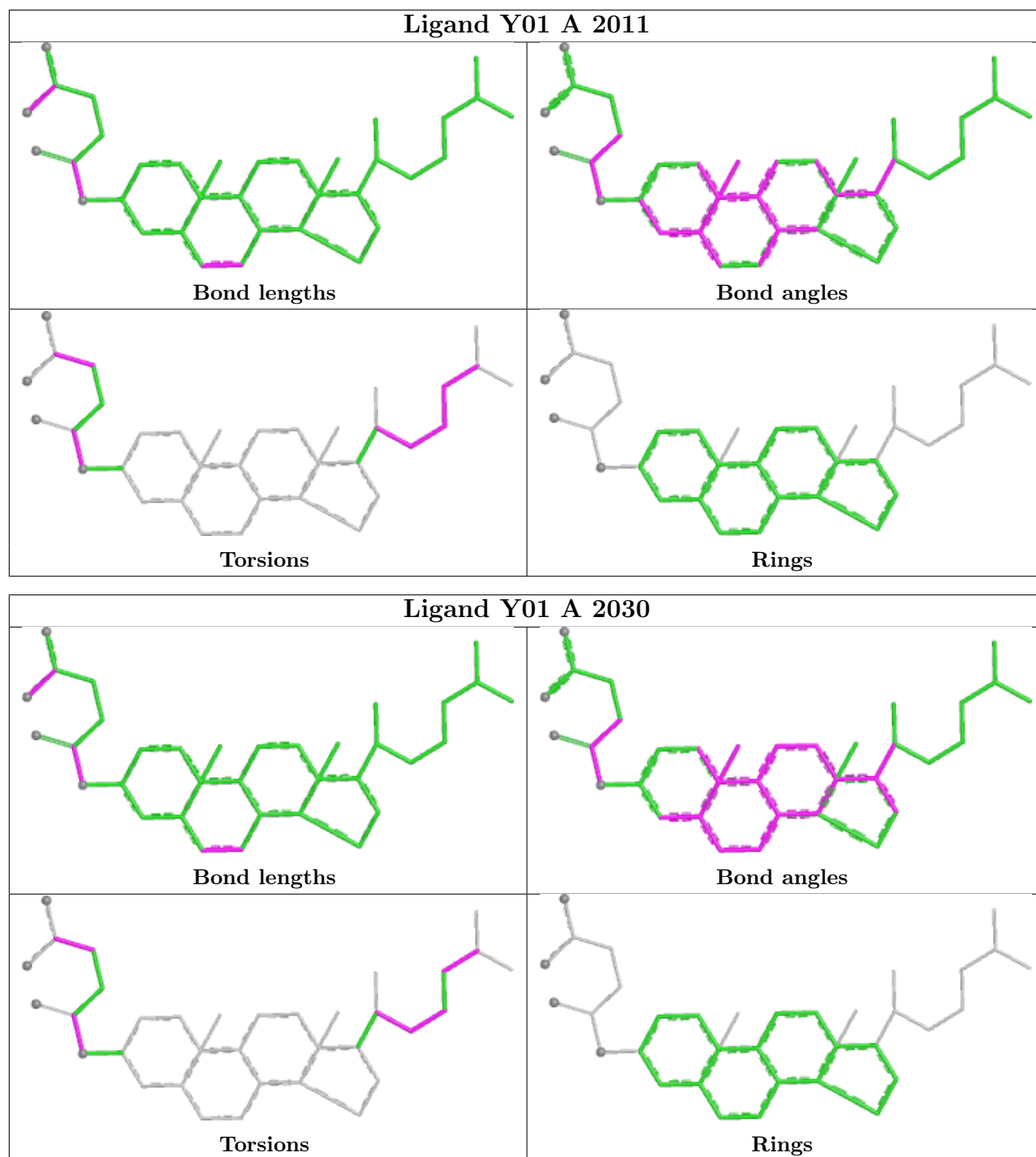
There are no ring outliers.

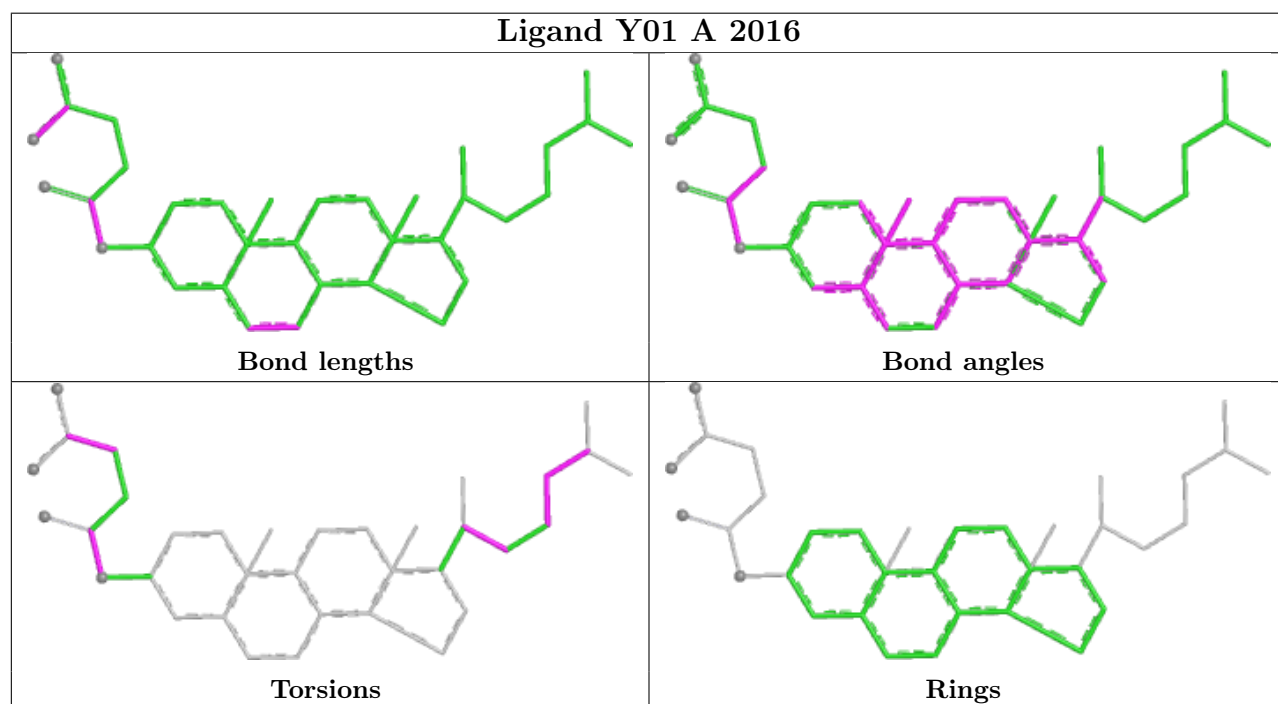
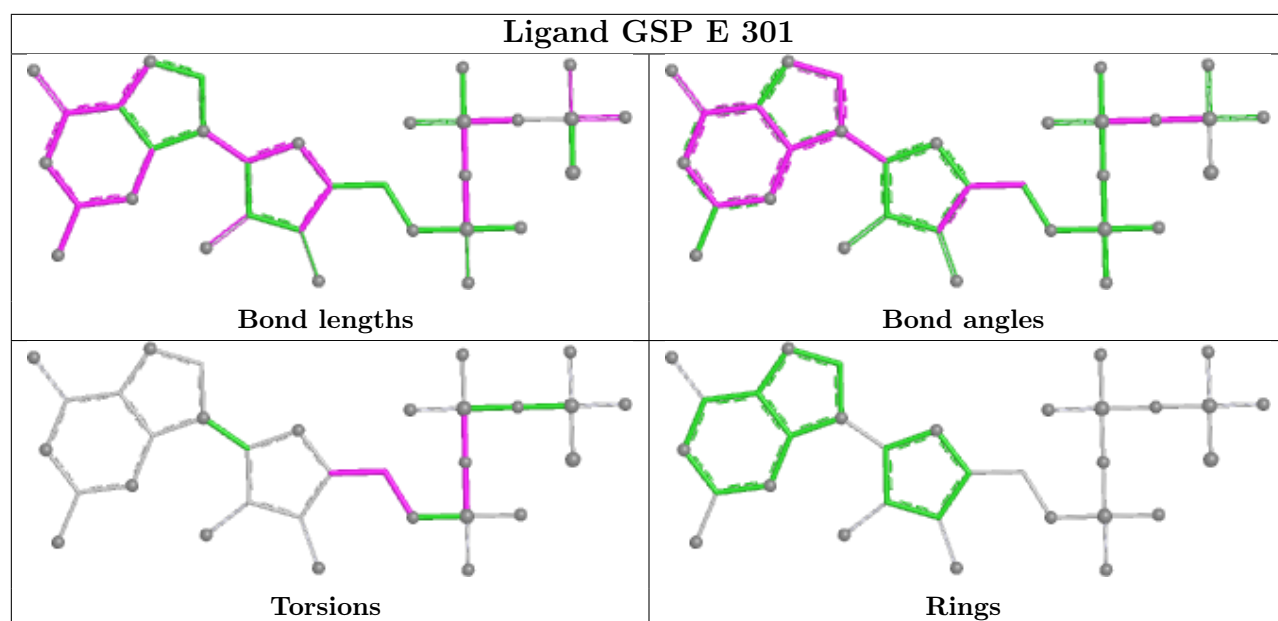
30 monomers are involved in 203 short contacts:

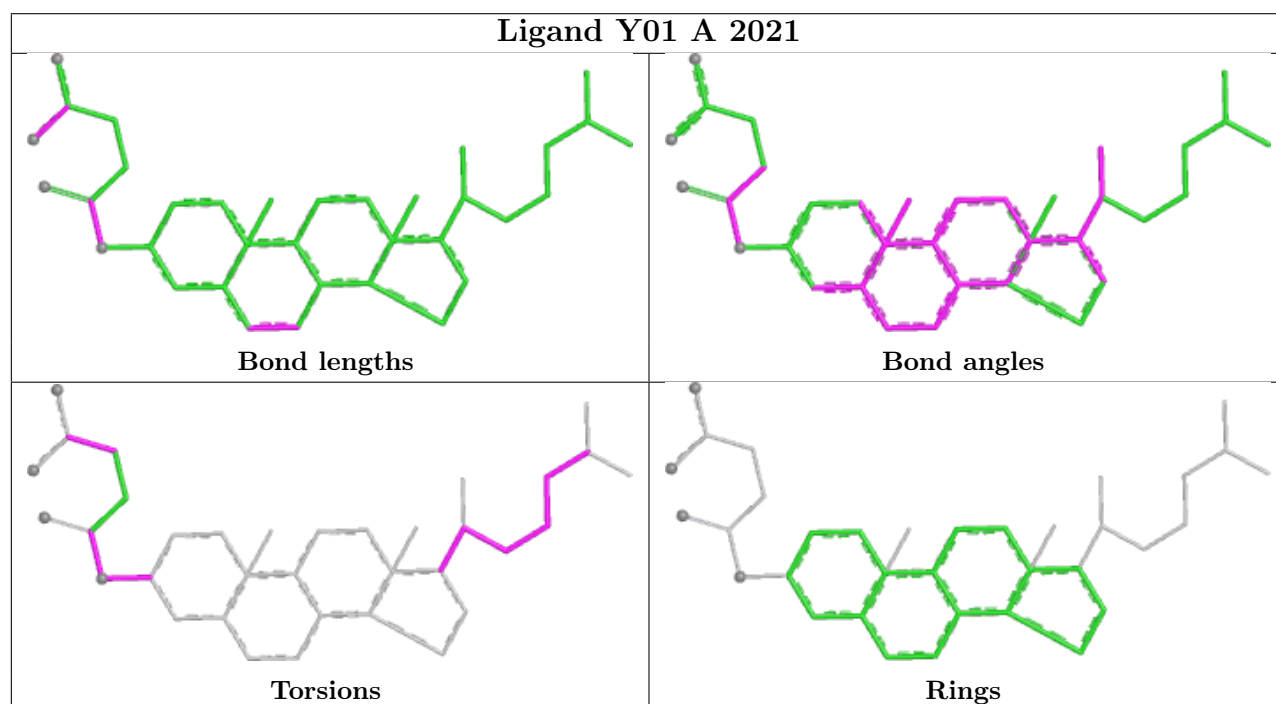
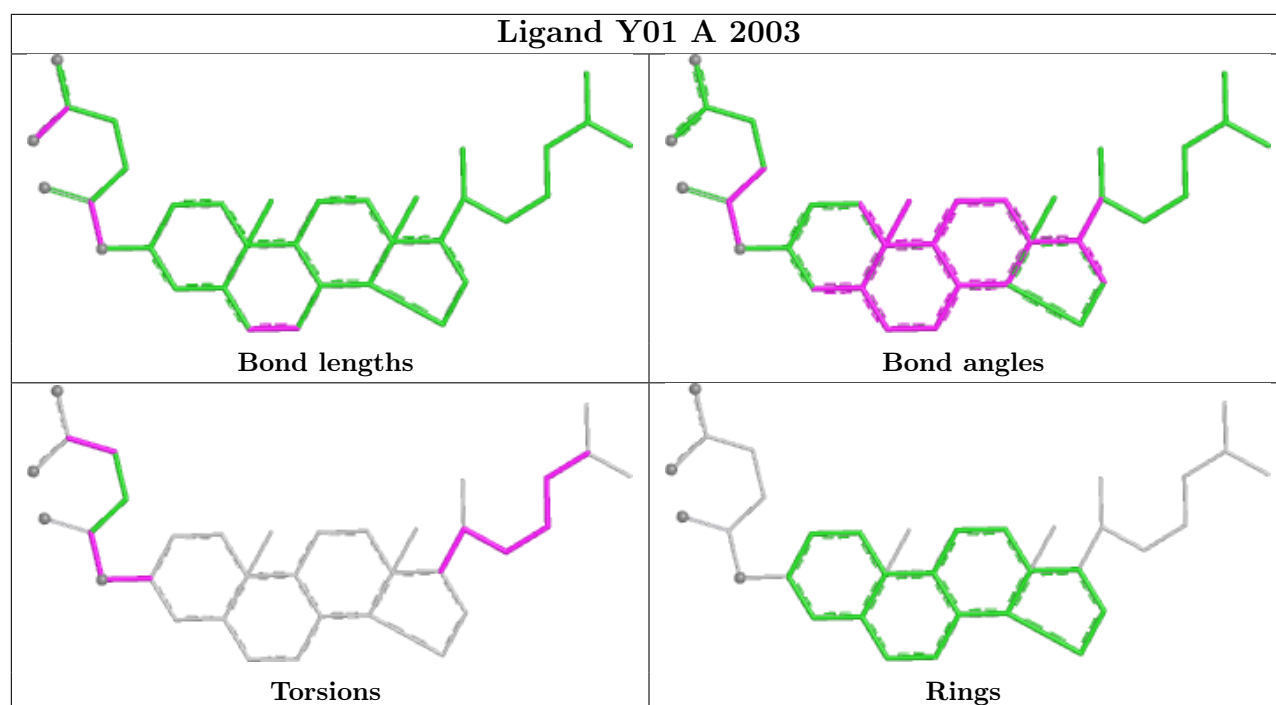
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2011	Y01	6	0
8	A	2030	Y01	5	0
8	A	2016	Y01	9	0
8	A	2003	Y01	13	0
8	A	2021	Y01	5	0
8	A	2029	Y01	7	0
8	A	2004	Y01	2	0
8	A	2019	Y01	7	0
8	A	2027	Y01	6	0
8	A	2026	Y01	5	0
9	A	2006	3PE	2	0
8	A	2009	Y01	9	0
8	A	2024	Y01	7	0
8	A	2020	Y01	13	0
8	A	2015	Y01	9	0
8	A	2008	Y01	10	0
8	A	2017	Y01	7	0
8	A	2010	Y01	12	0
8	A	2002	Y01	9	0
8	A	2022	Y01	10	0
8	A	2028	Y01	5	0
8	A	2013	Y01	9	0
8	A	2007	Y01	8	0
8	A	2012	Y01	12	0
8	H	102	Y01	7	0
8	A	2014	Y01	12	0
8	A	2025	Y01	6	0
8	A	2023	Y01	9	0
8	A	2018	Y01	13	0
8	A	2005	Y01	11	0

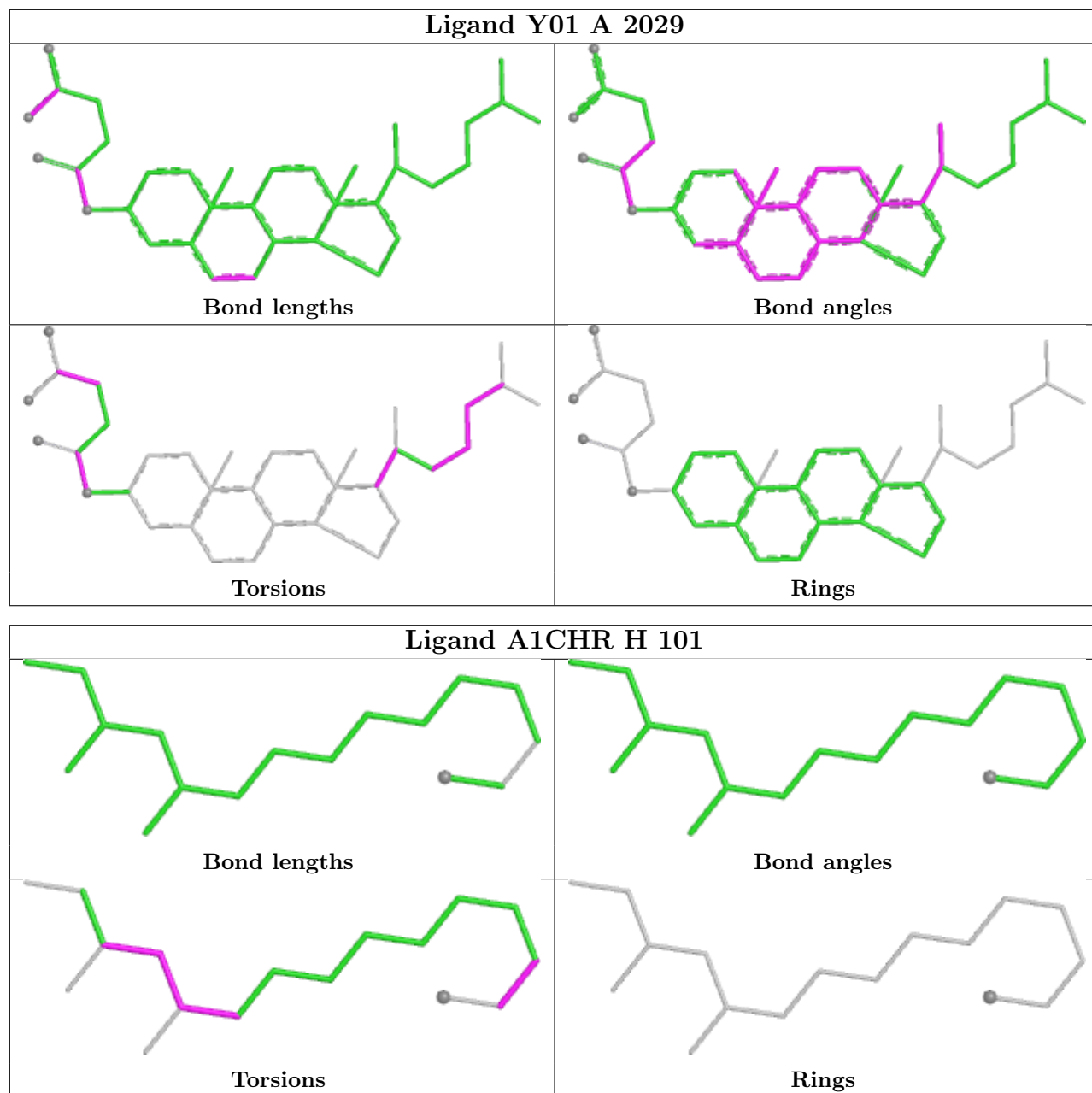
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

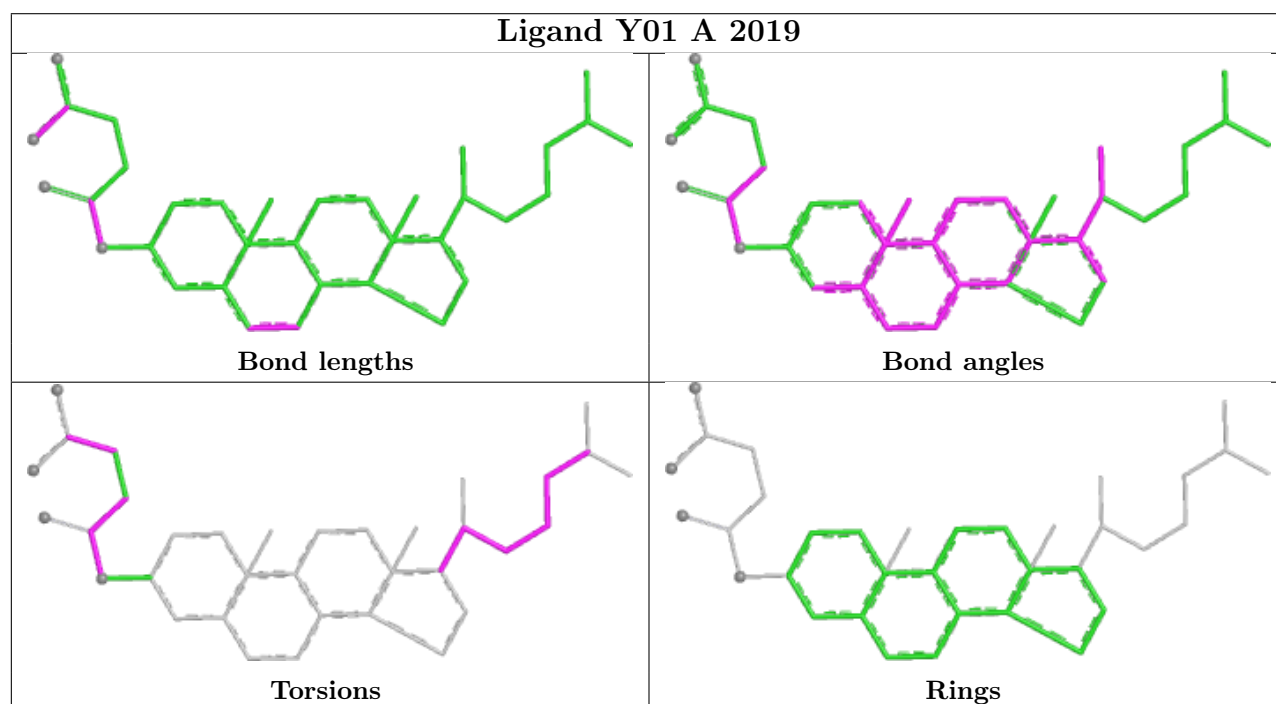
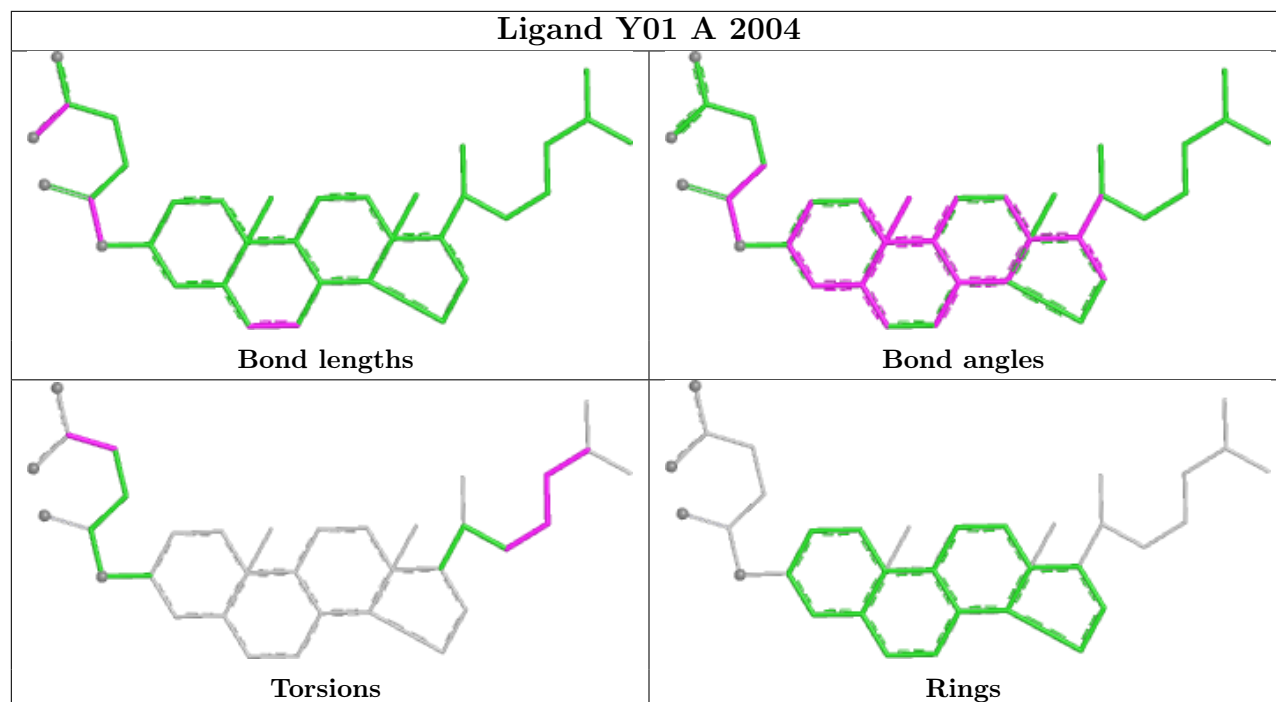
equivalents in the CSD to analyse the geometry.

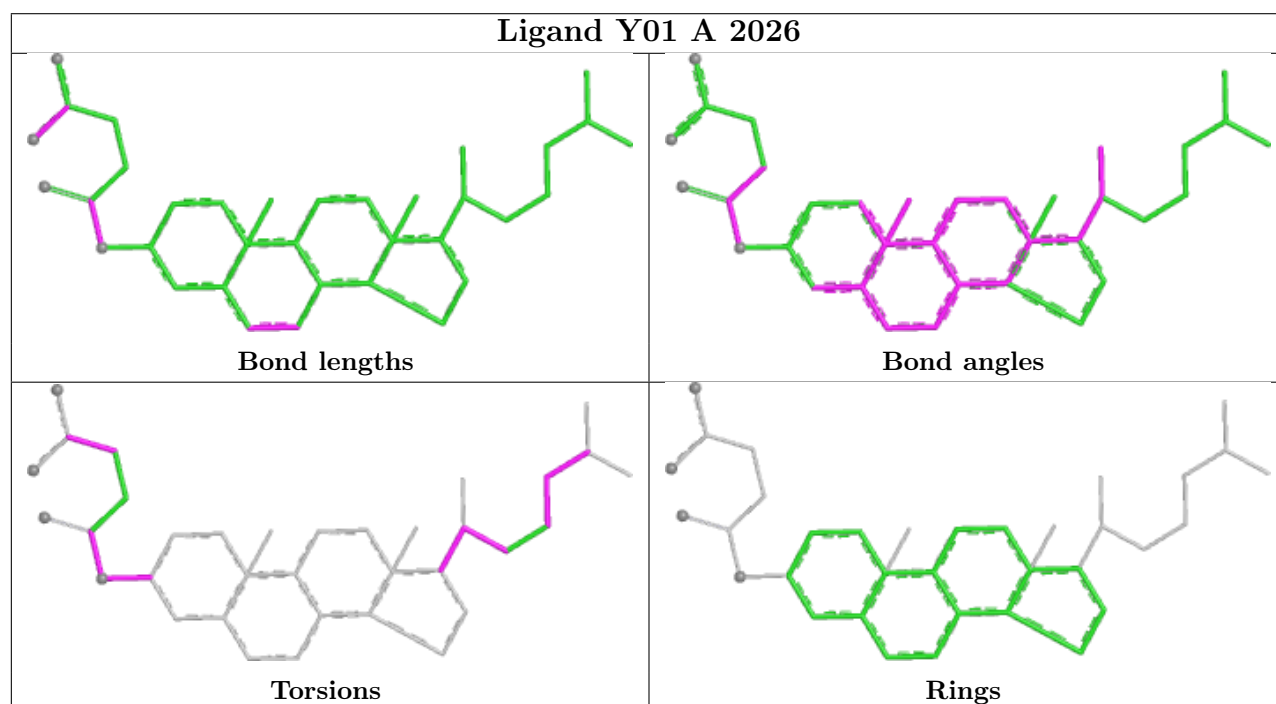
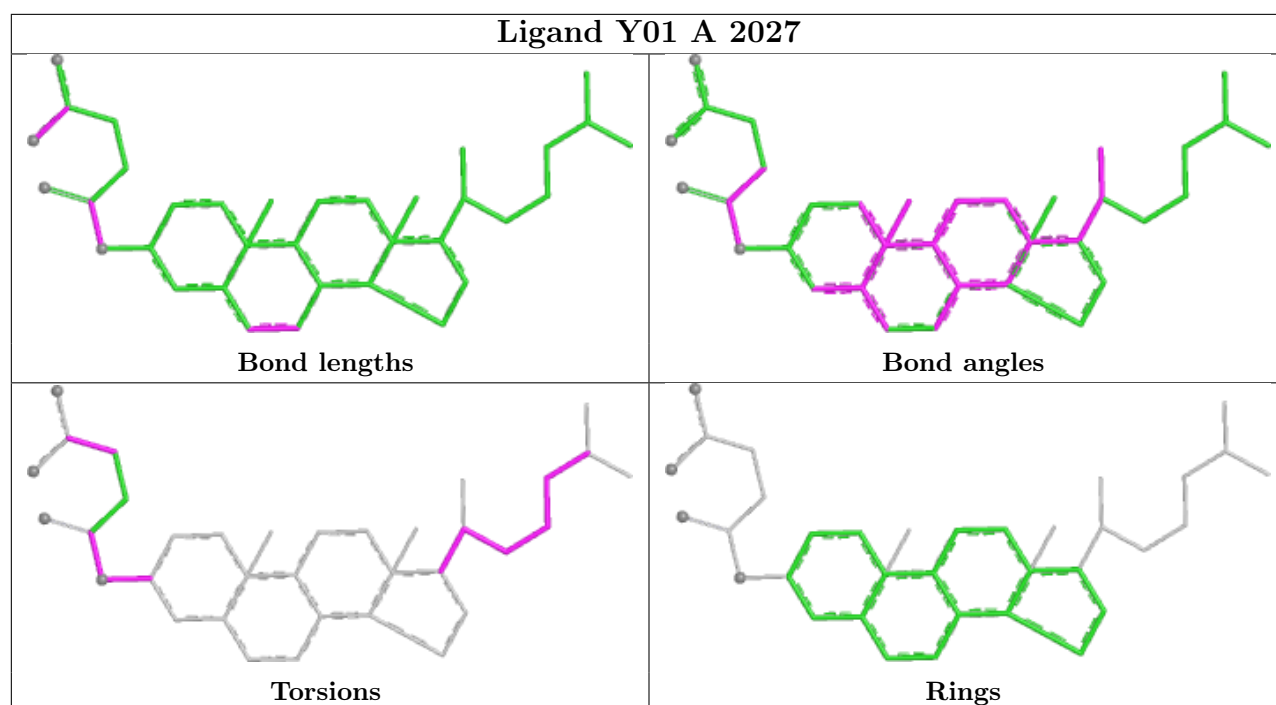


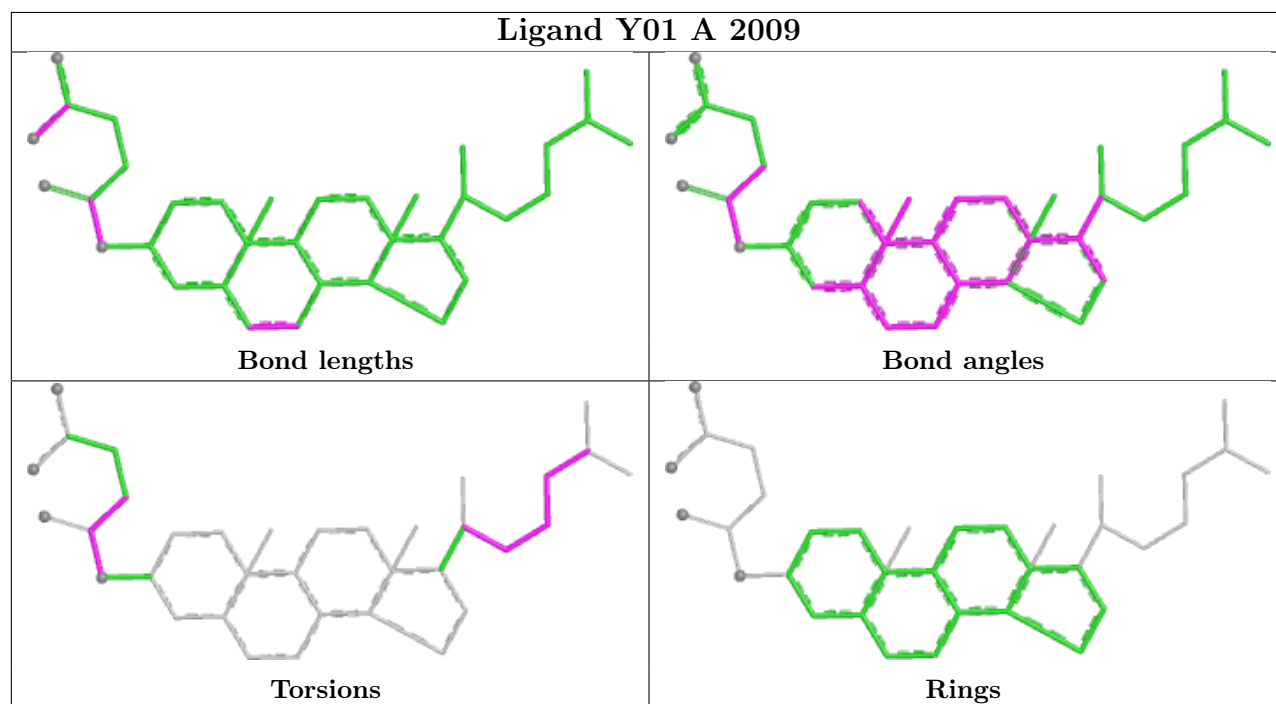
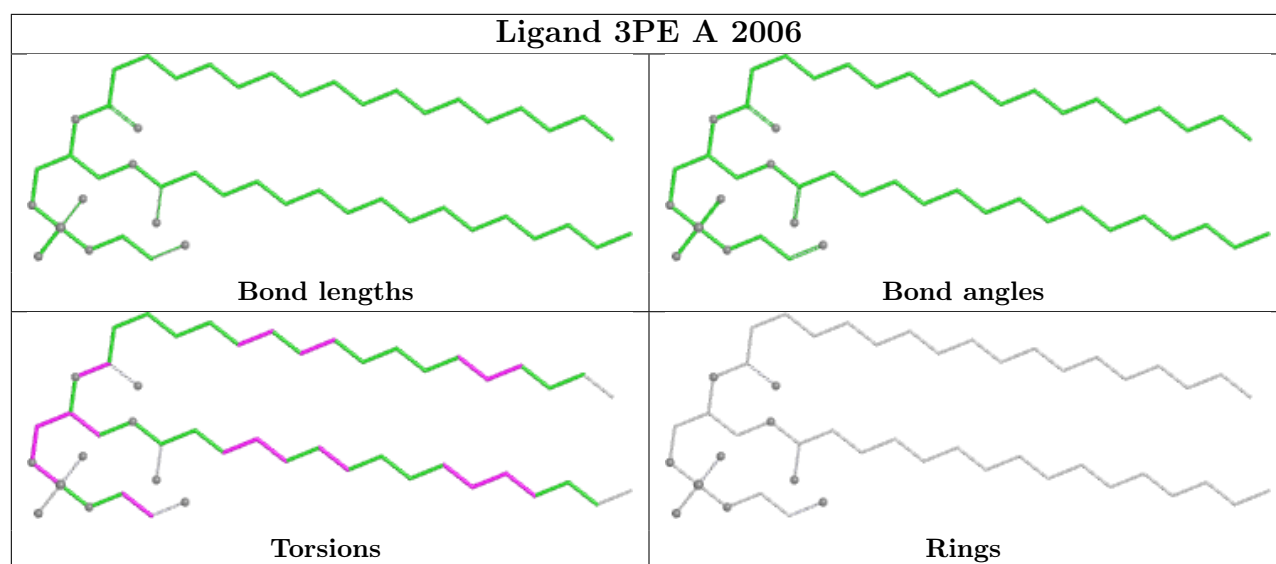


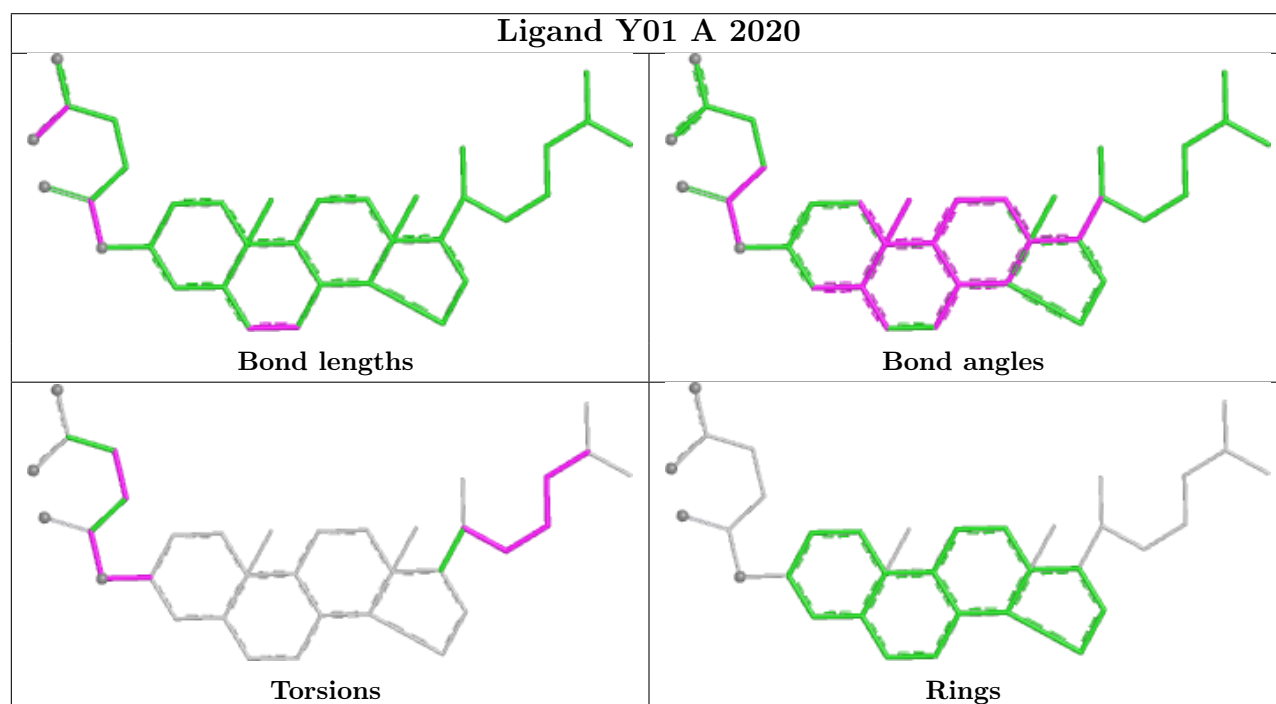
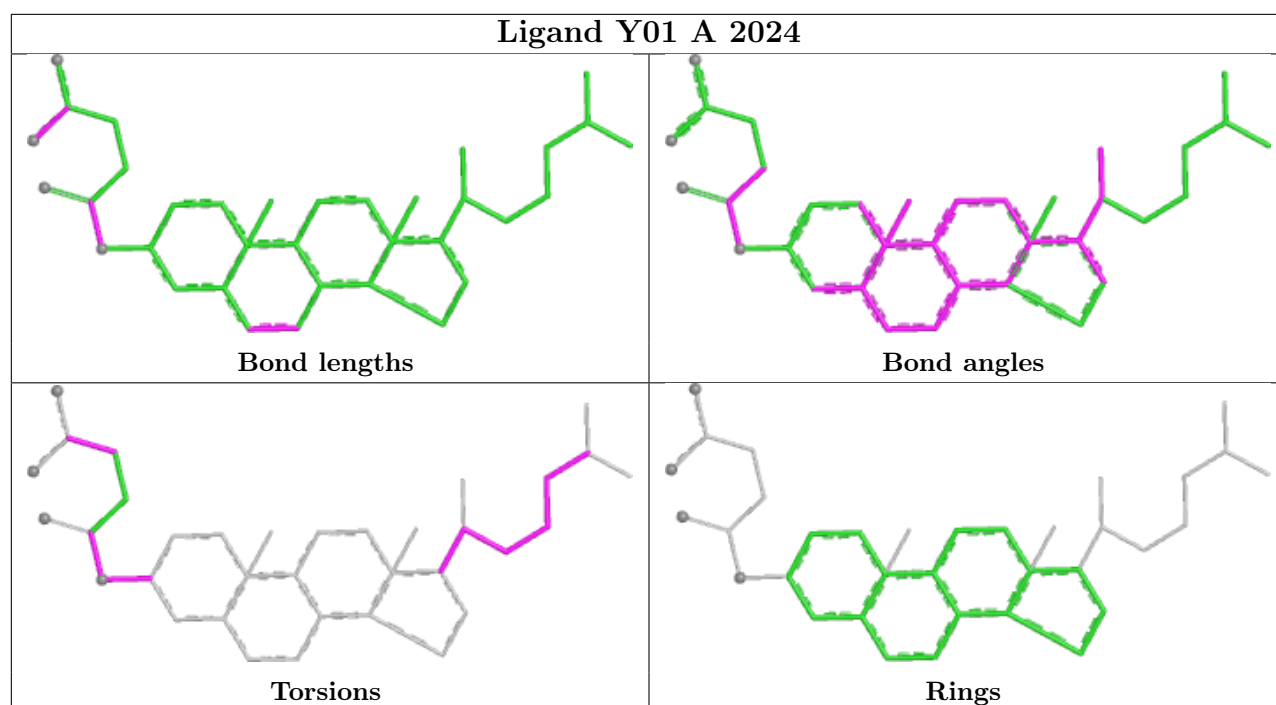


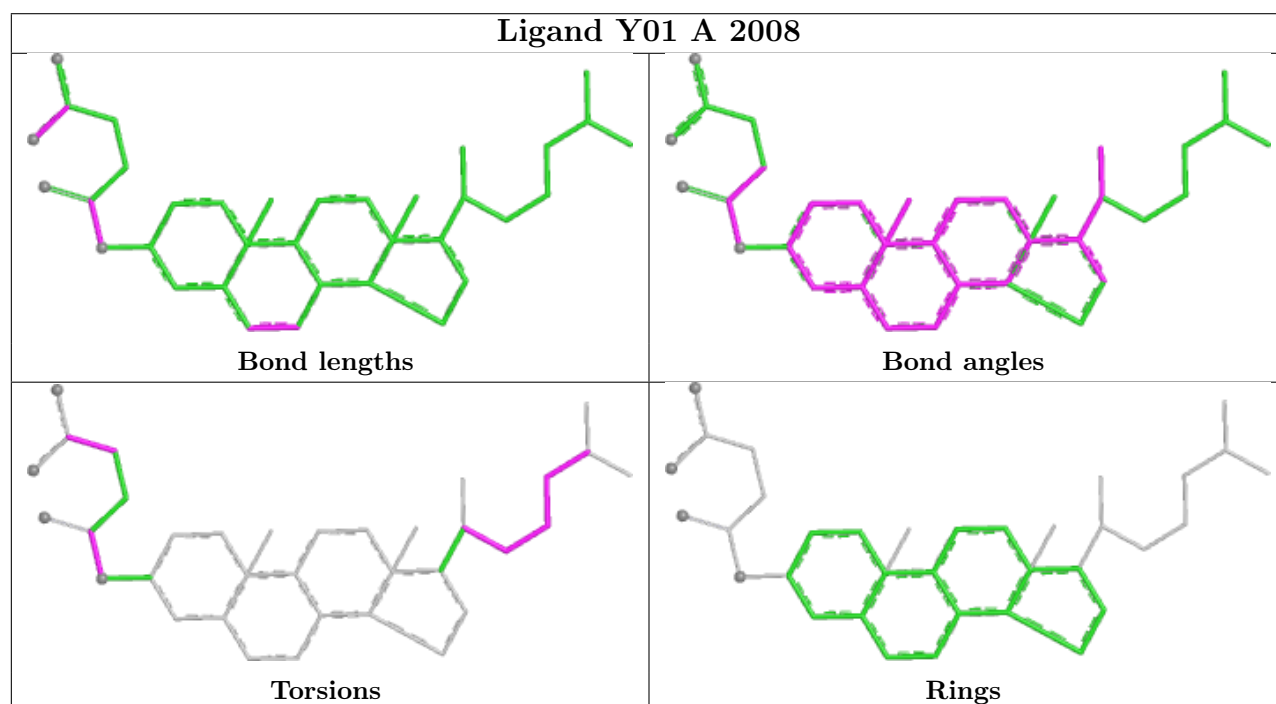
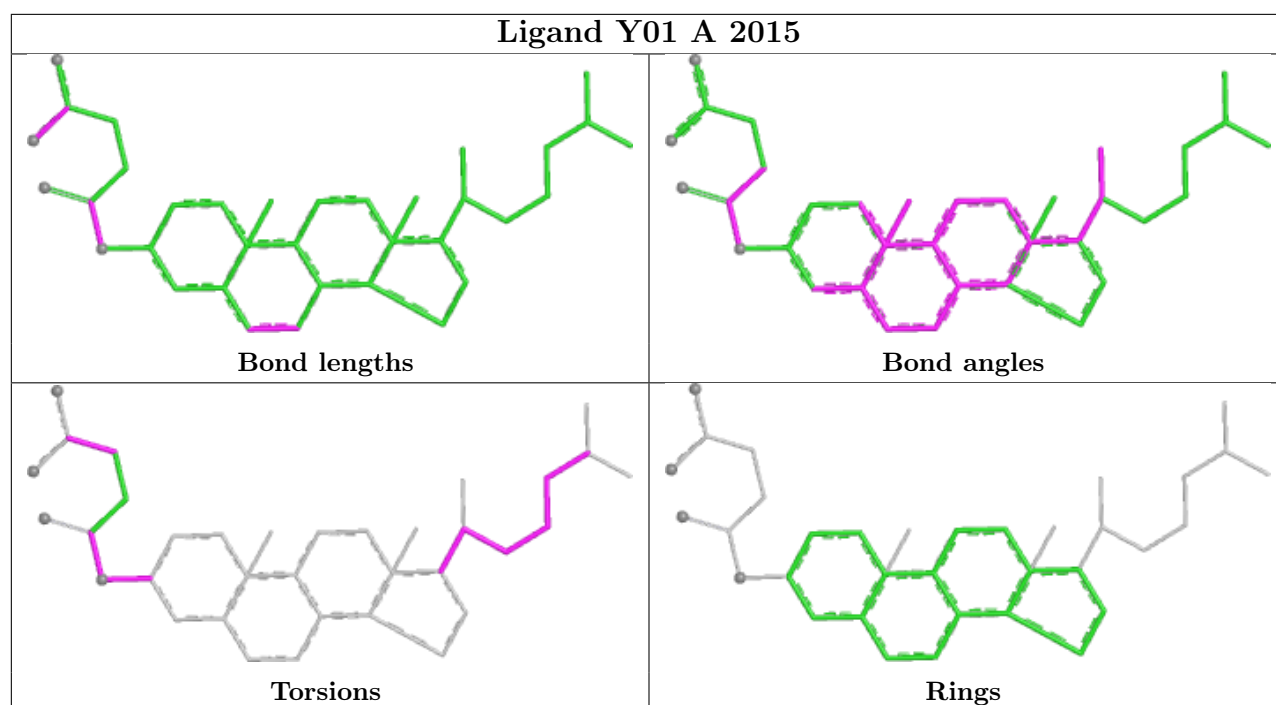


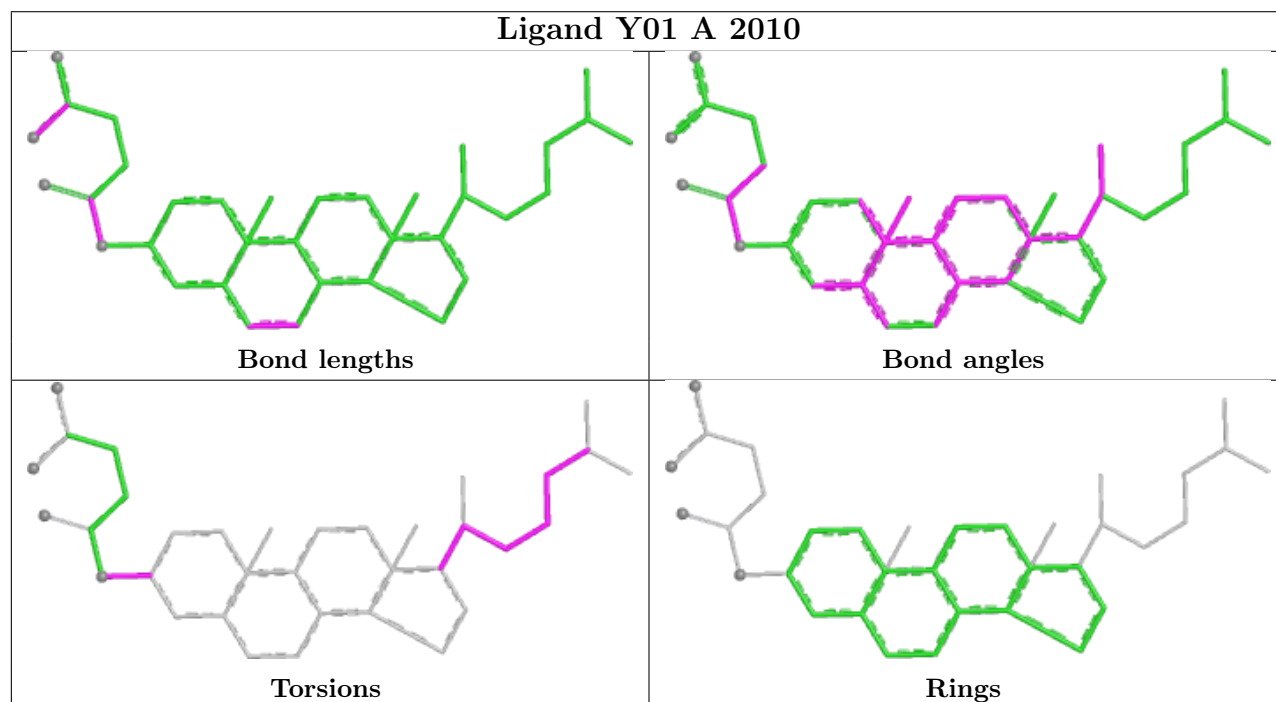
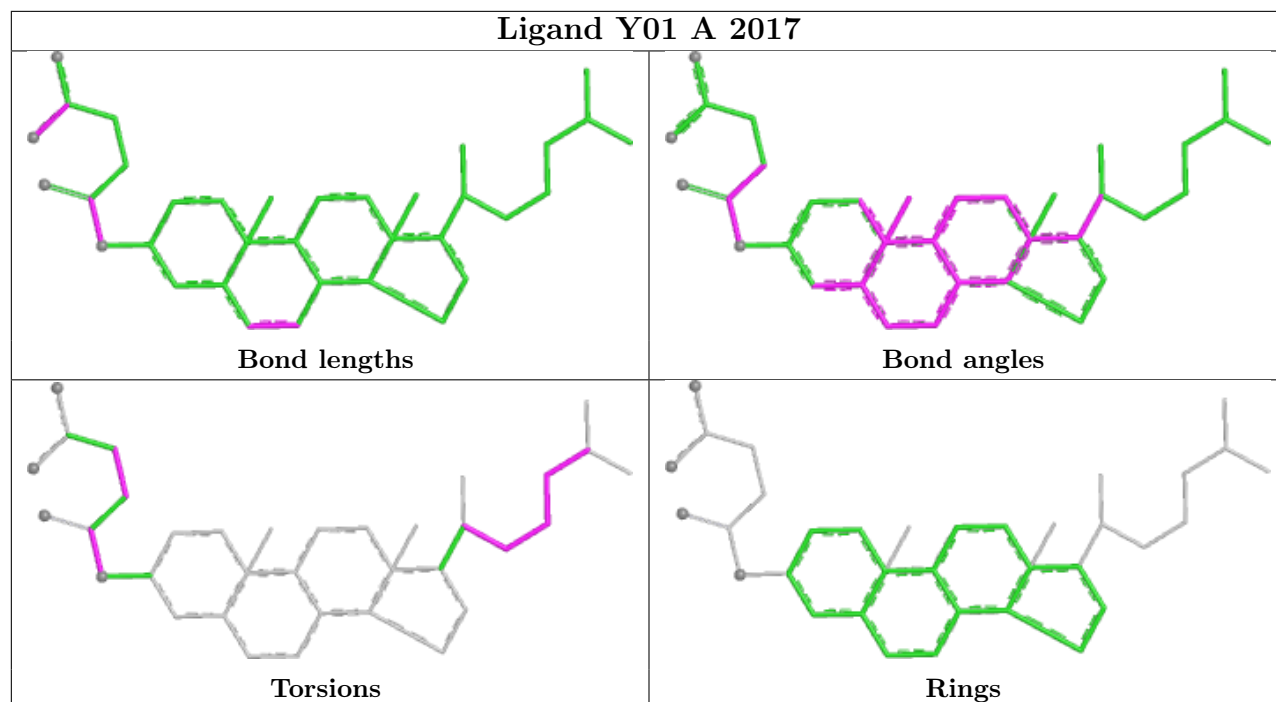


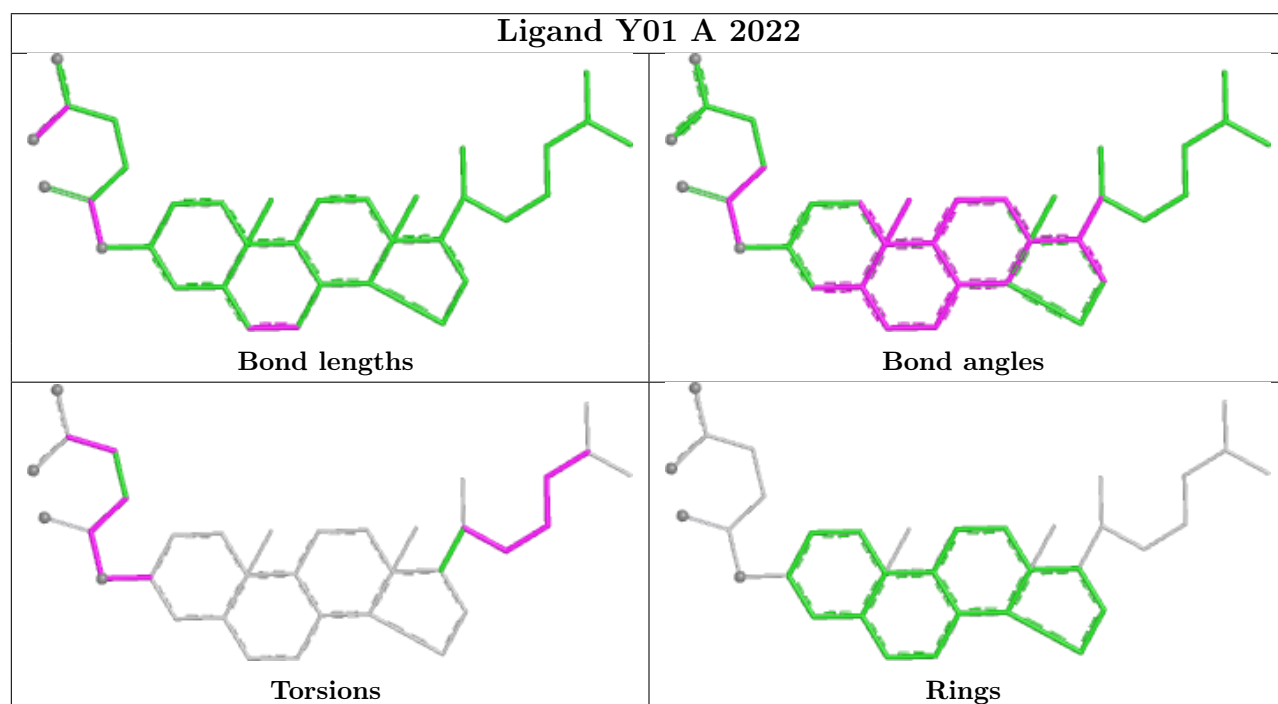
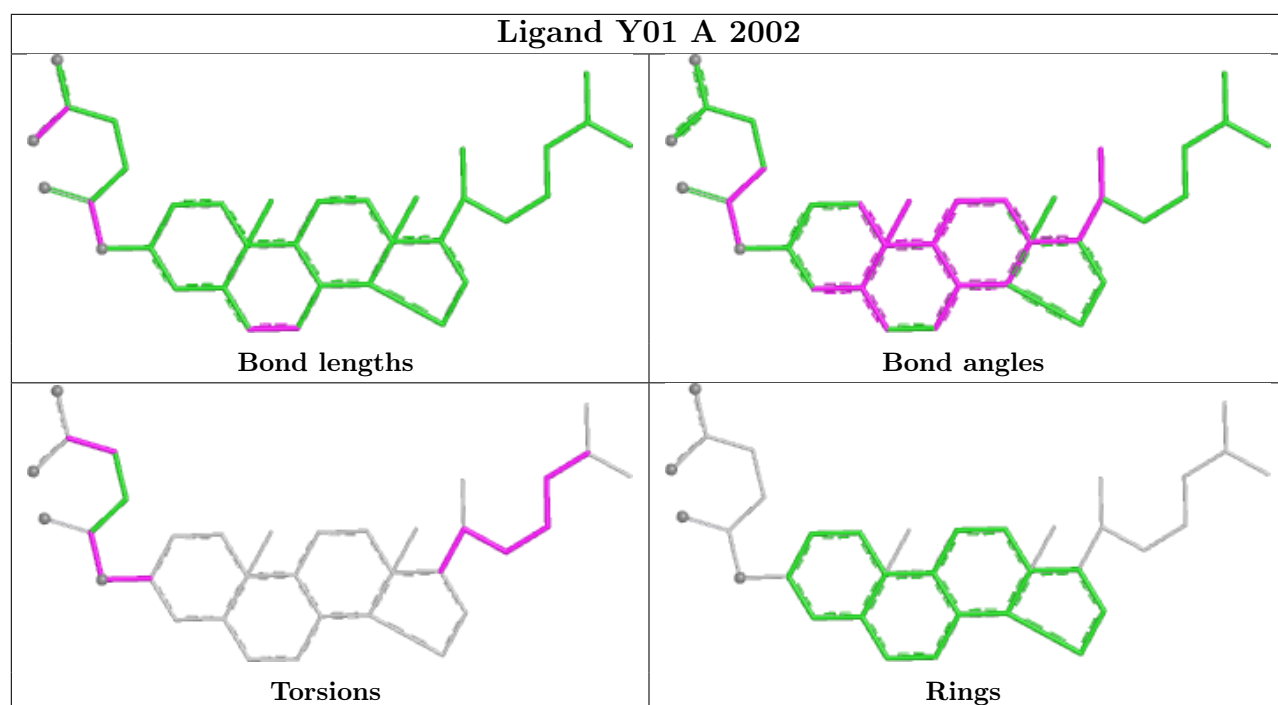


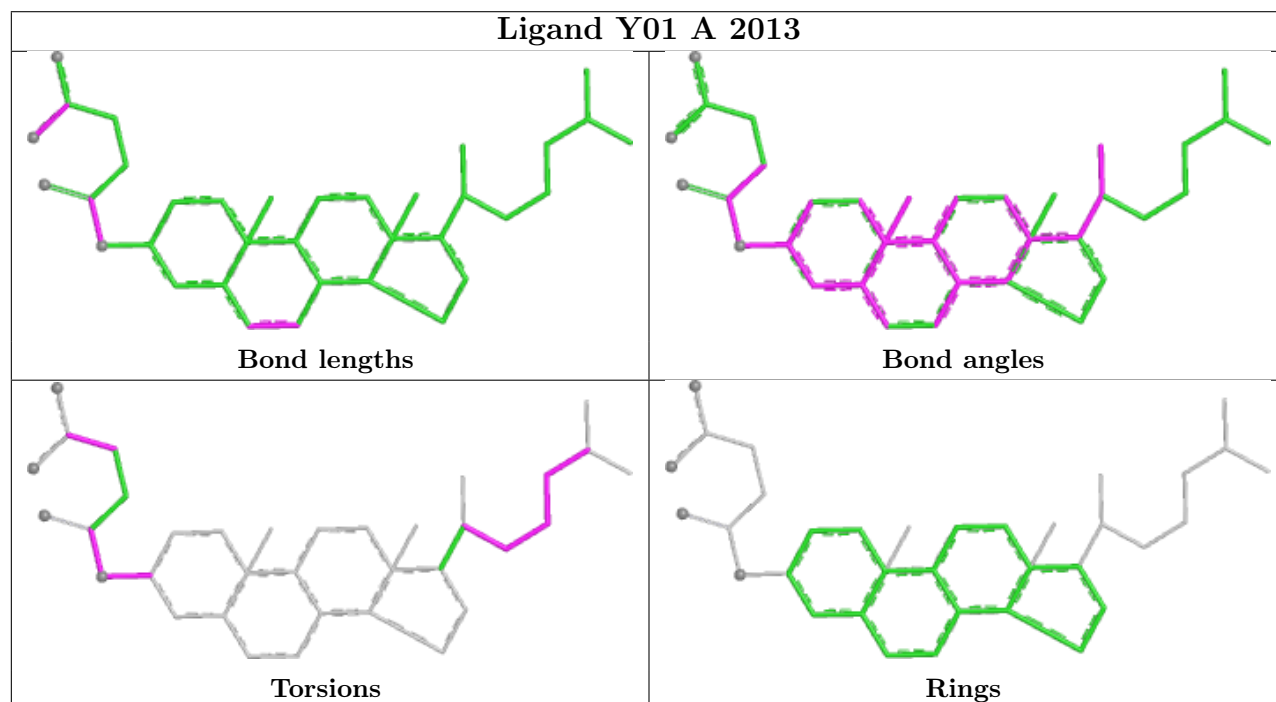
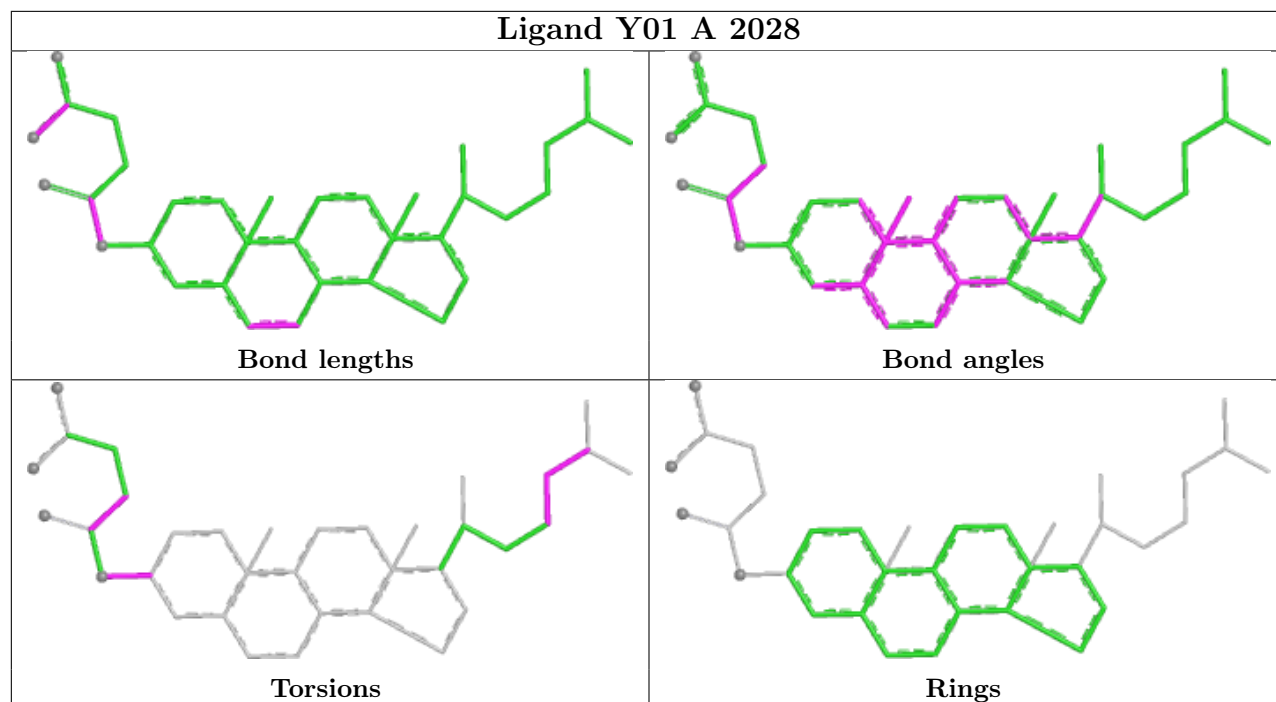


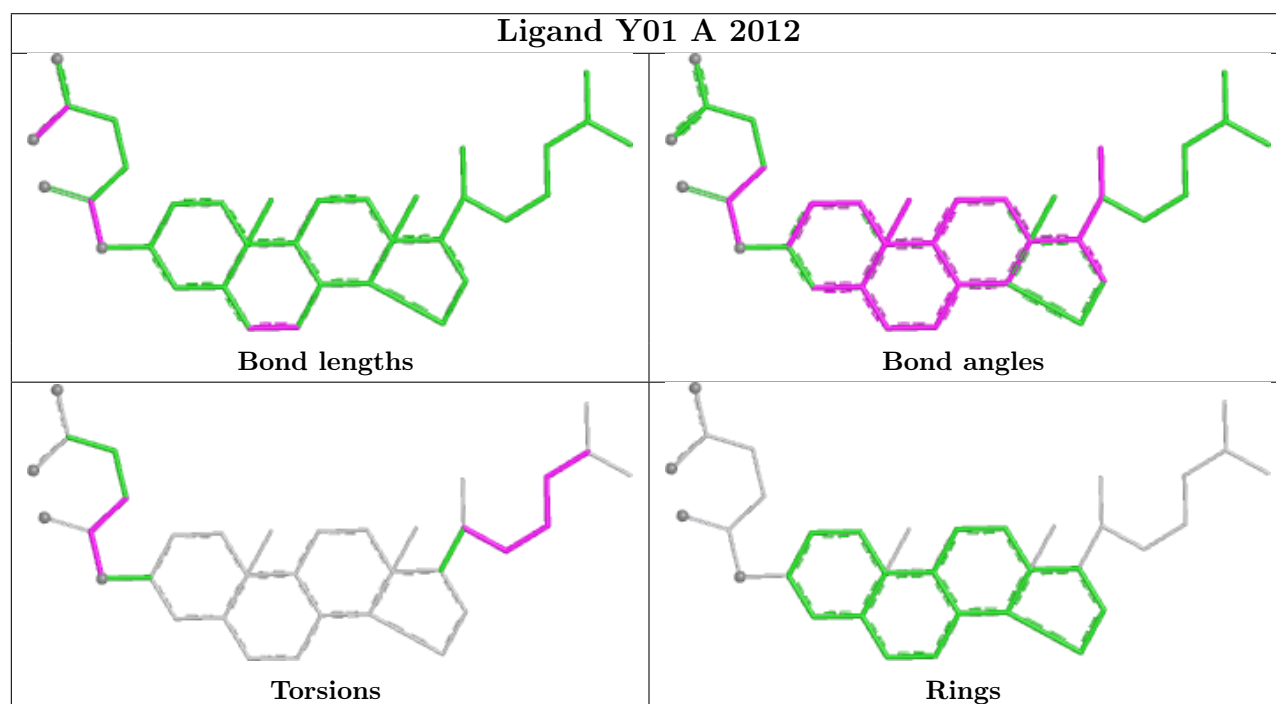
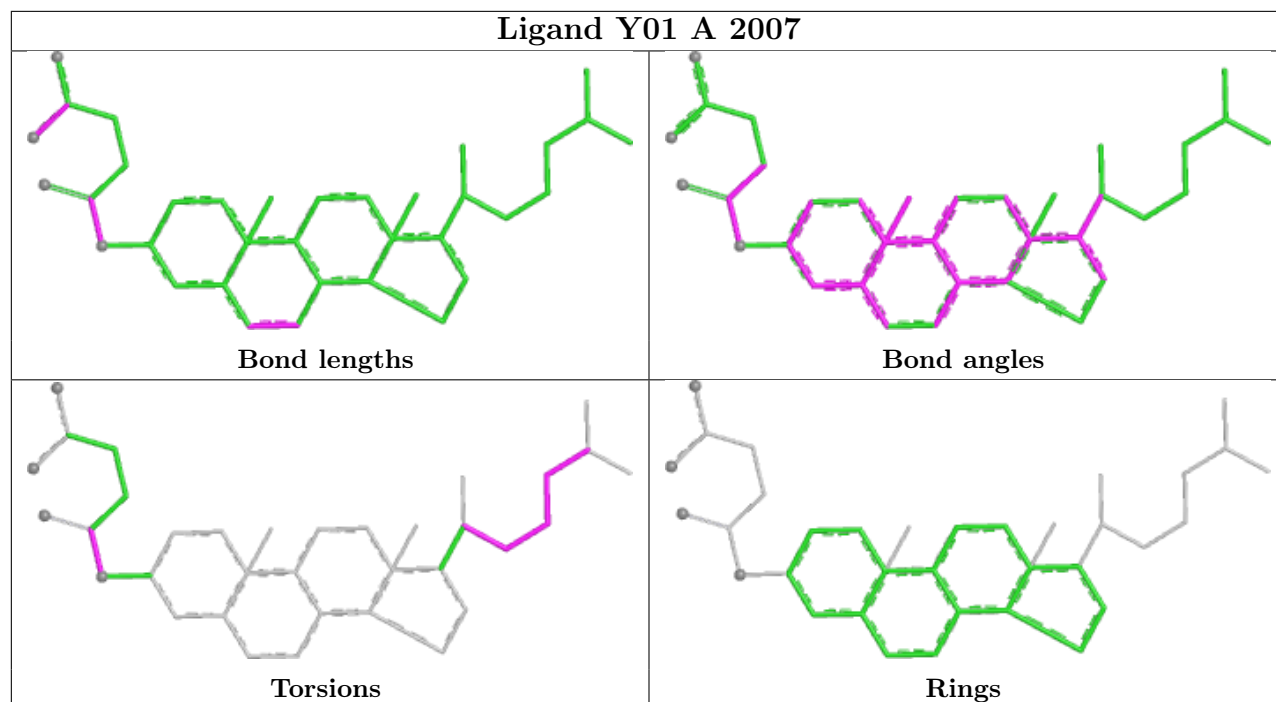


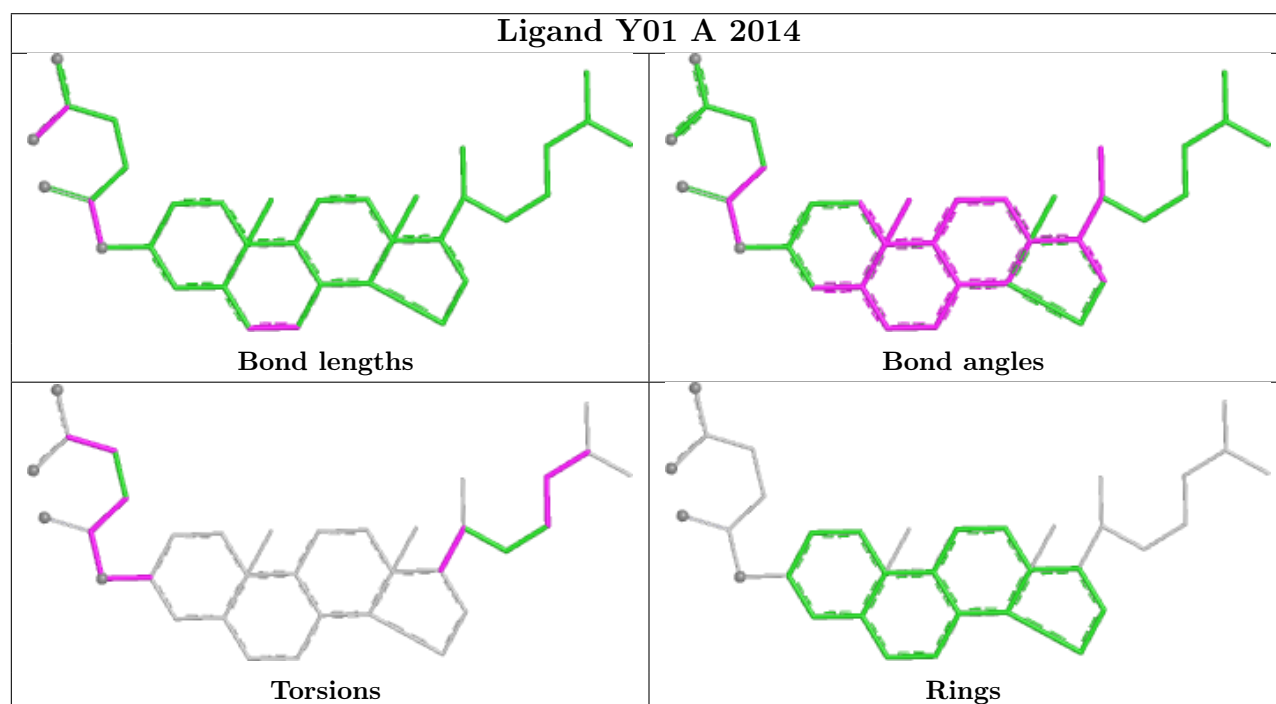
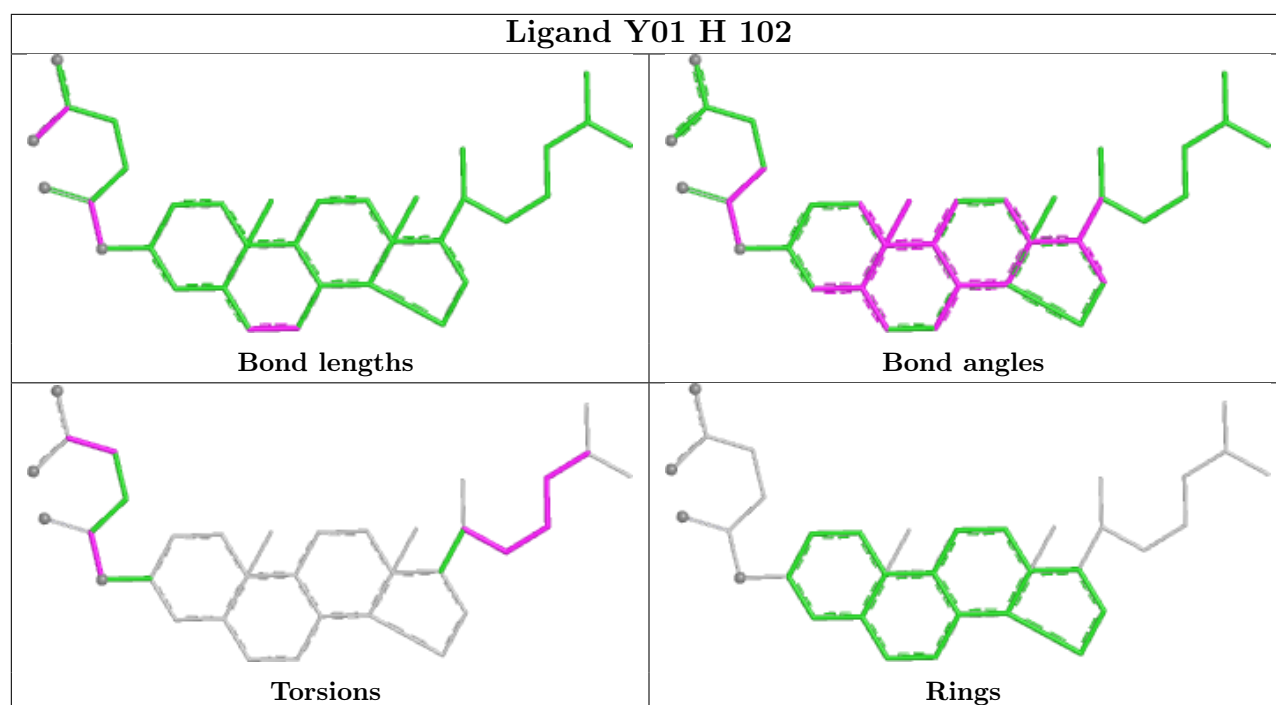


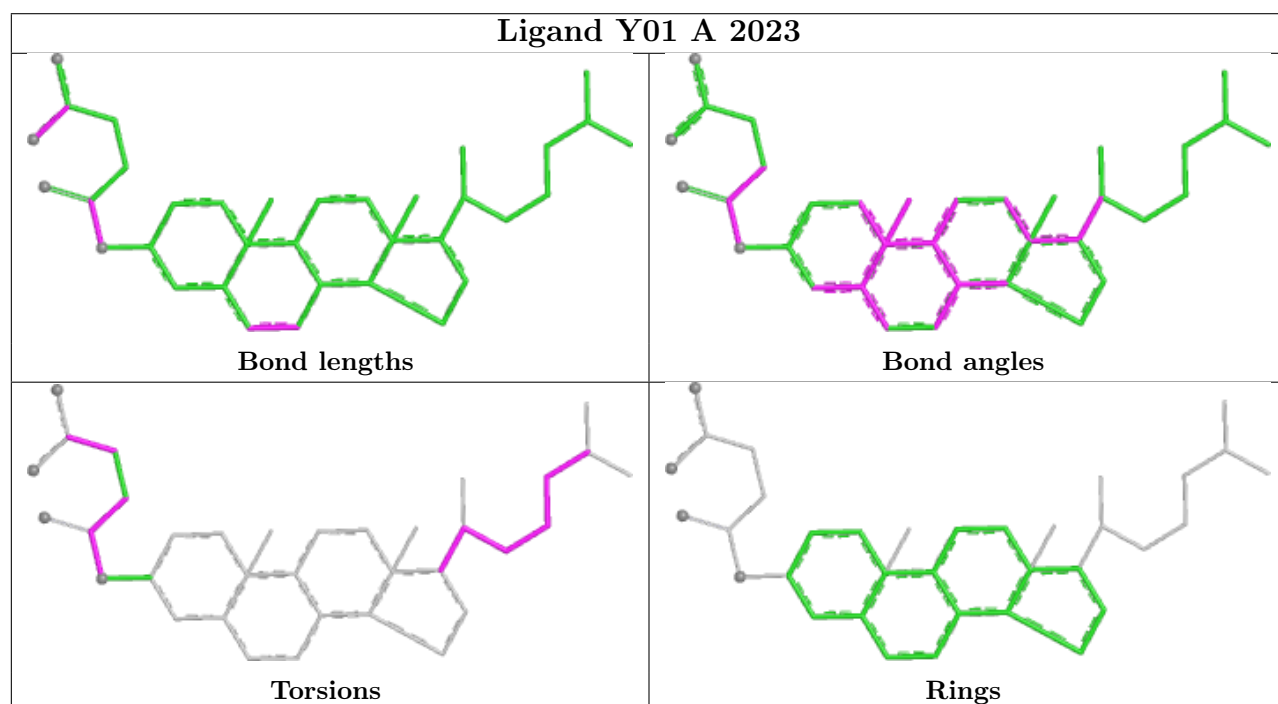
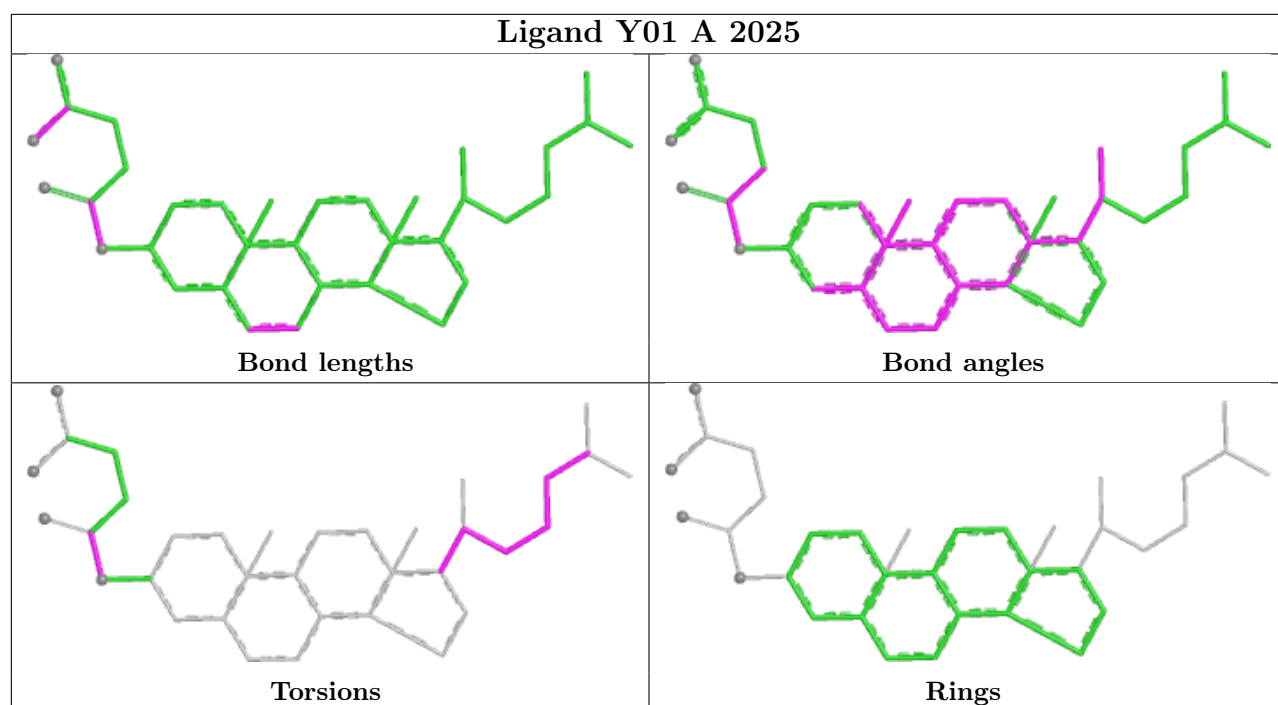


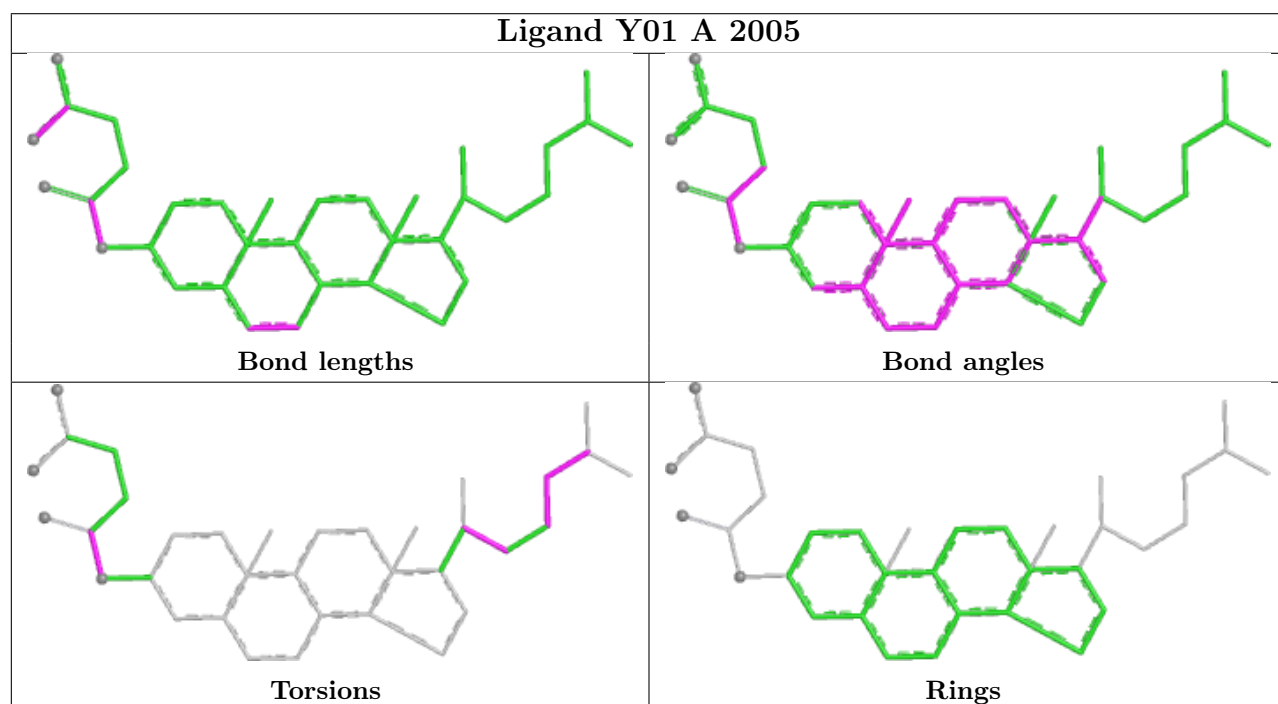
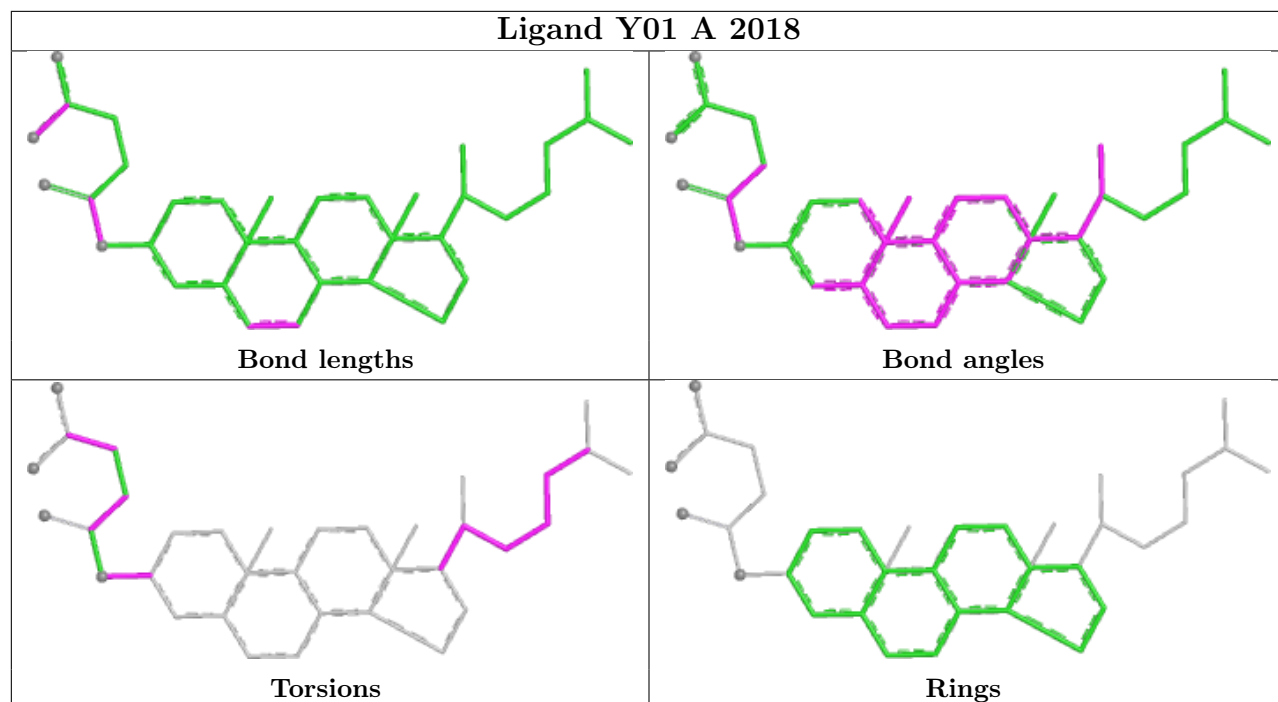


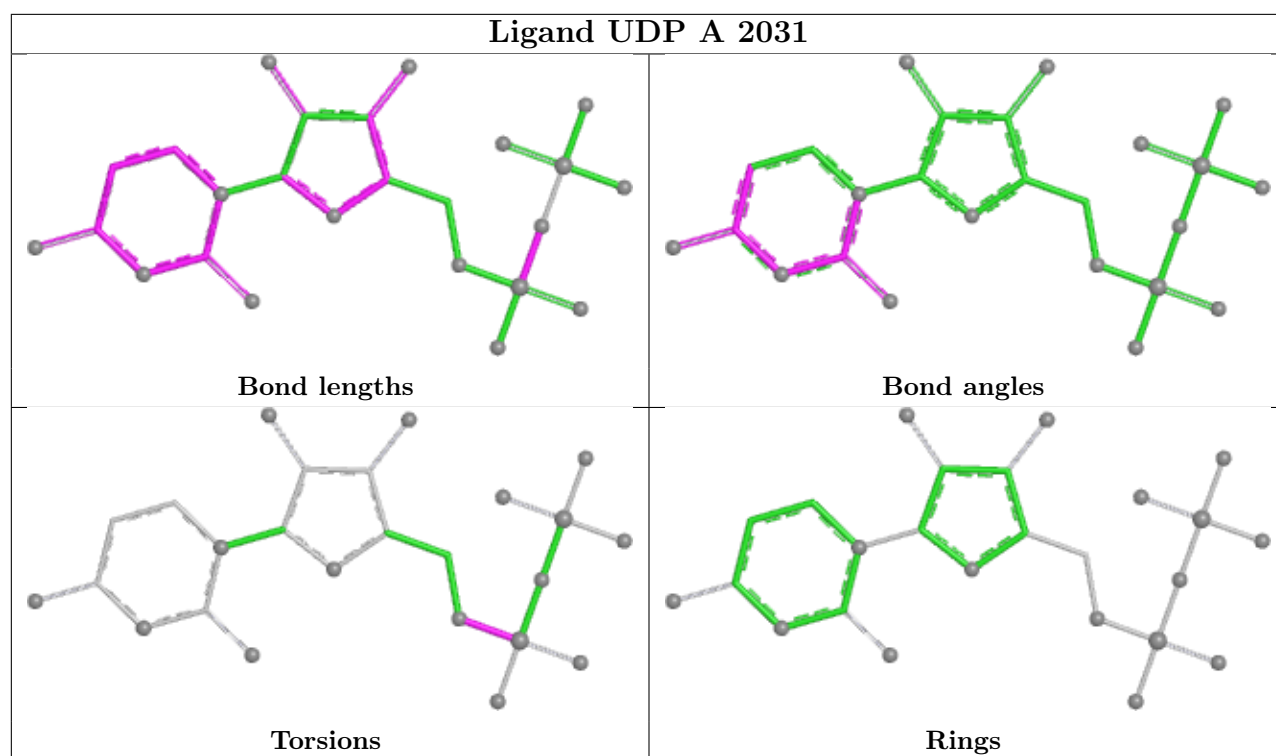












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

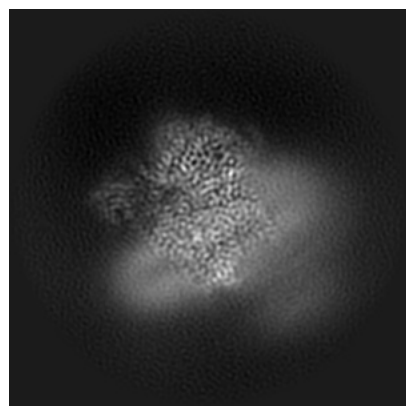
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71550. These allow visual inspection of the internal detail of the map and identification of artifacts.

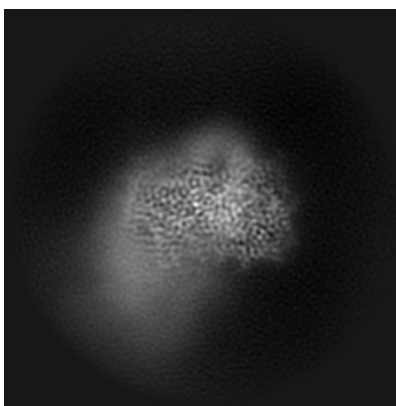
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

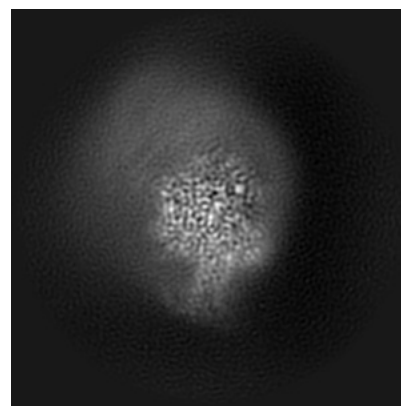
6.1.1 Primary map



X

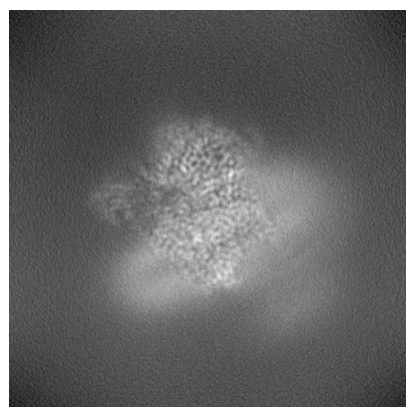


Y

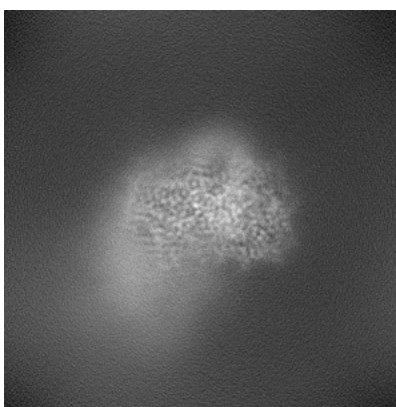


Z

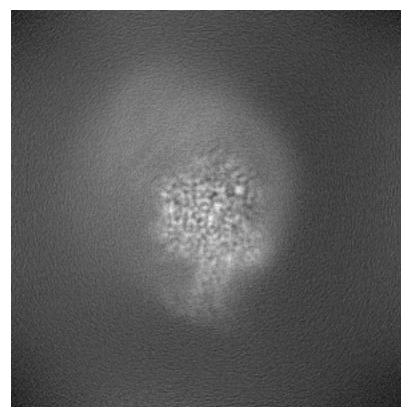
6.1.2 Raw map



X



Y

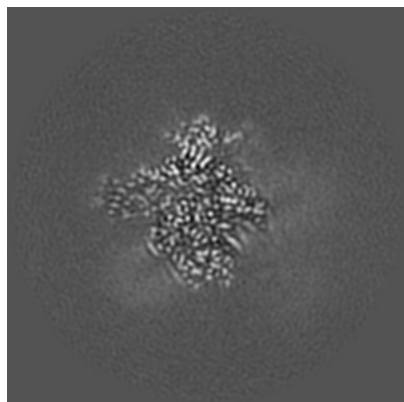


Z

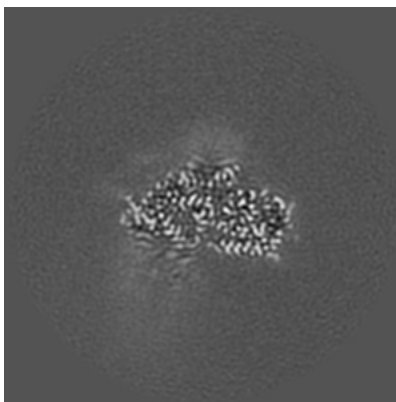
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

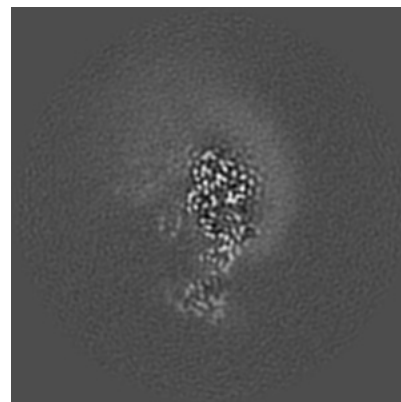
6.2.1 Primary map



X Index: 160

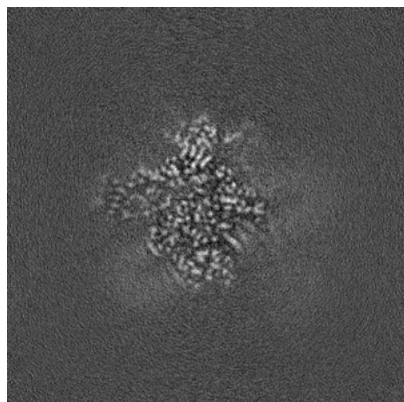


Y Index: 160

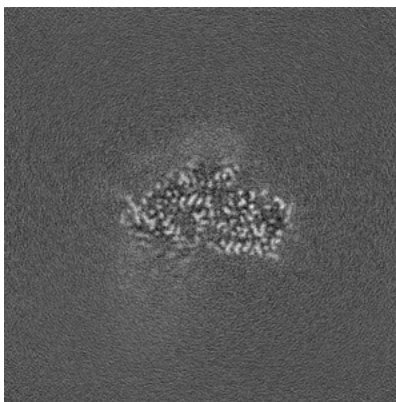


Z Index: 160

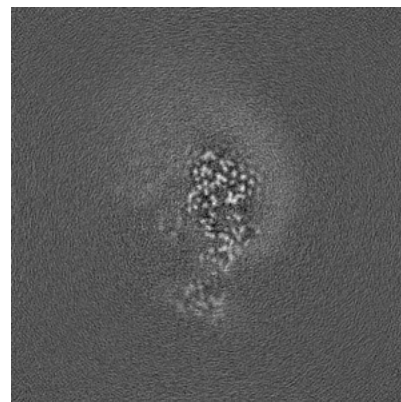
6.2.2 Raw map



X Index: 160



Y Index: 160

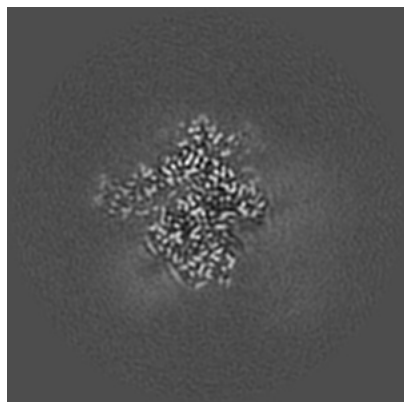


Z Index: 160

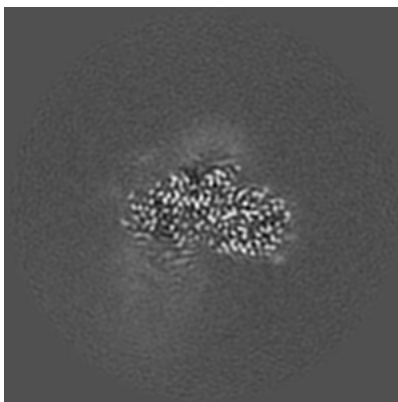
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

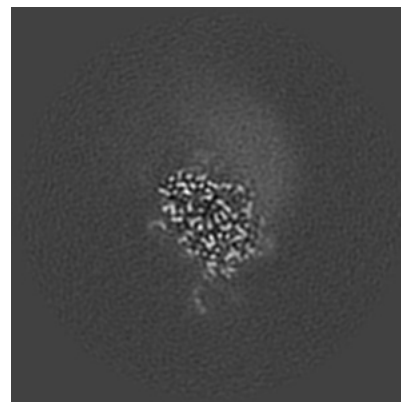
6.3.1 Primary map



X Index: 158

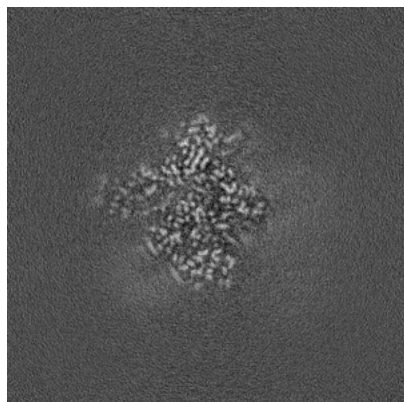


Y Index: 162

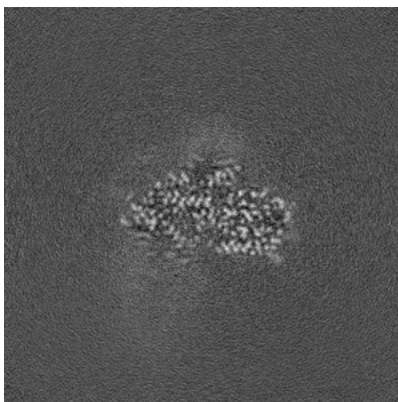


Z Index: 187

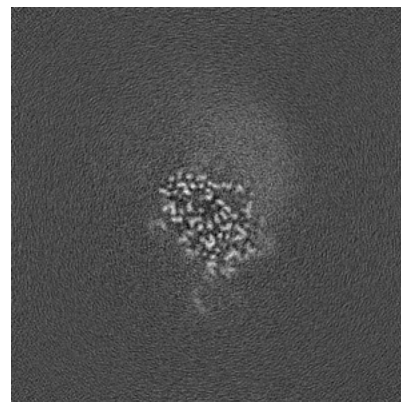
6.3.2 Raw map



X Index: 159



Y Index: 161

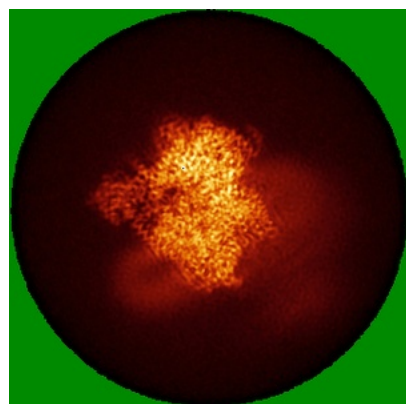


Z Index: 187

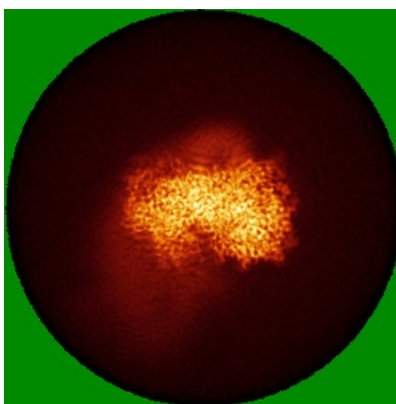
The images above show the largest variance slices of the map in three orthogonal directions.

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

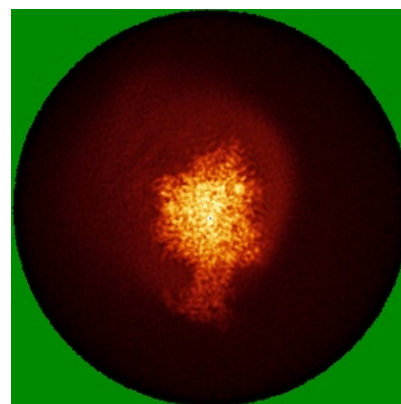
6.4.1 Primary map



X

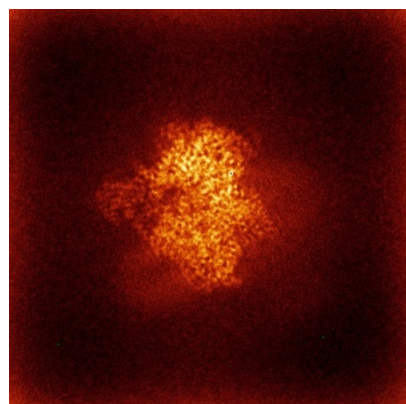


Y

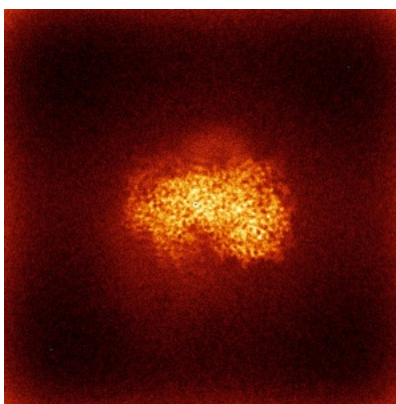


Z

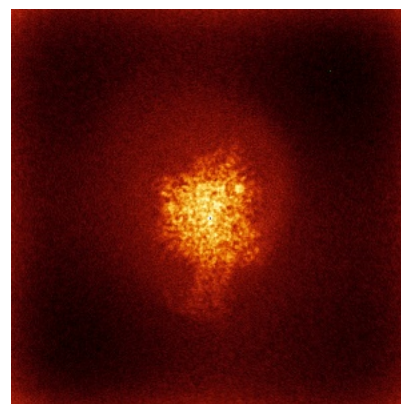
6.4.2 Raw map



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.

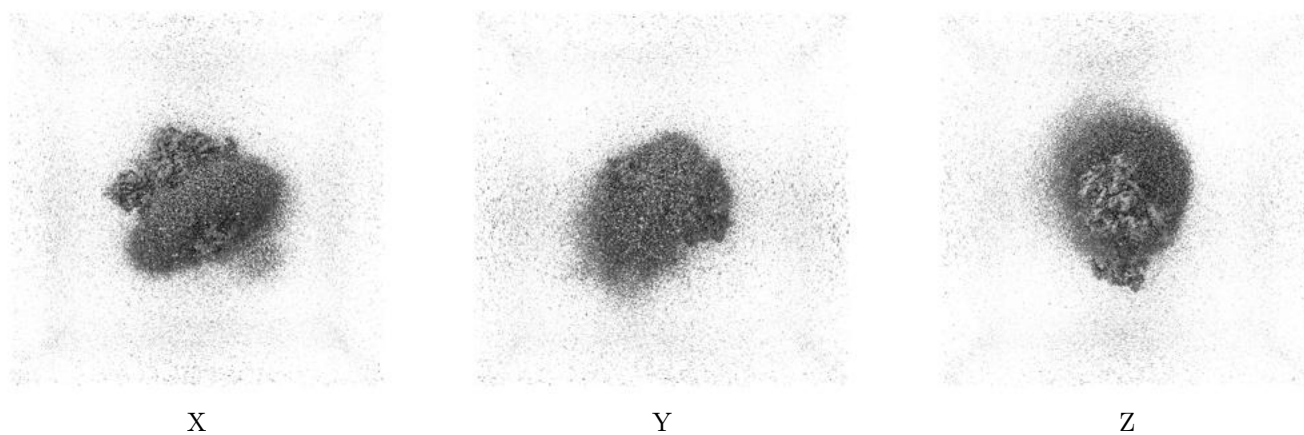
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0792. 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.

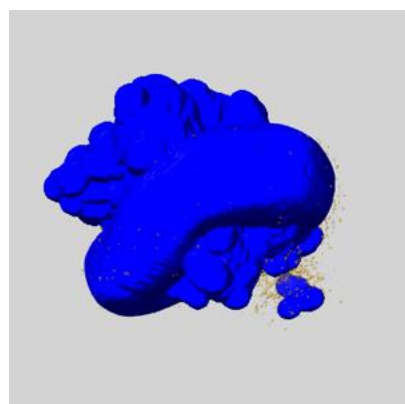
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

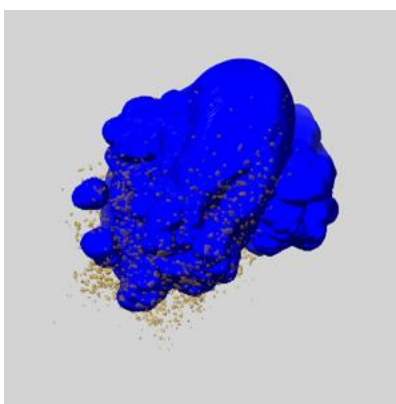
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

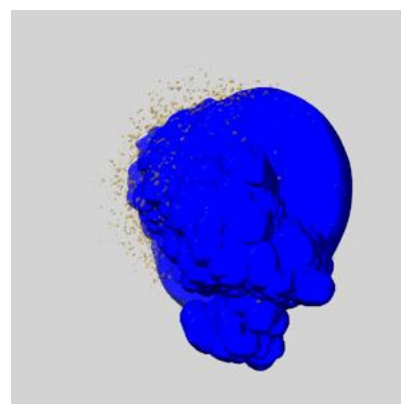
6.6.1 emd_71550_msk_1.map [i](#)



X



Y

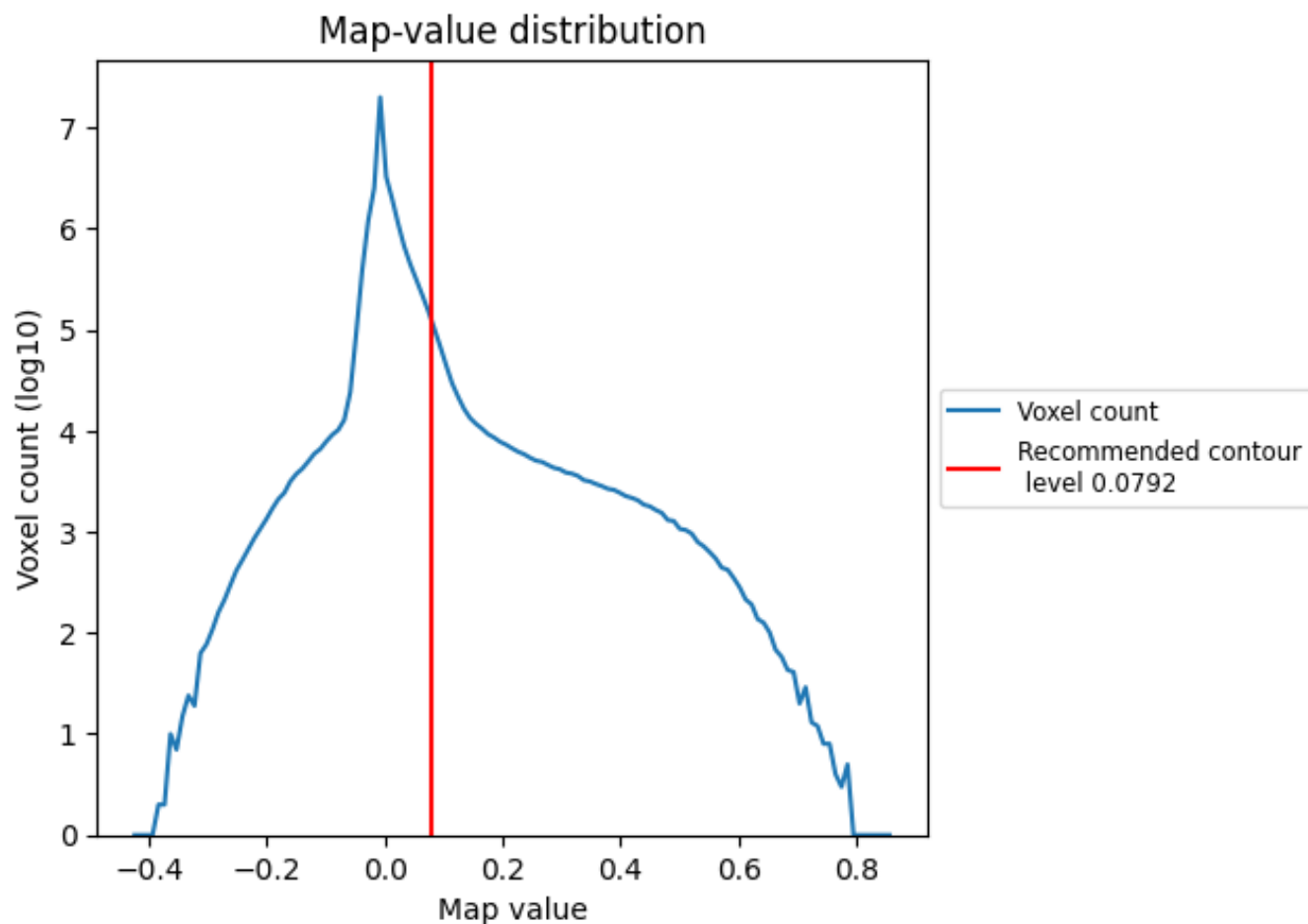


Z

7 Map analysis [i](#)

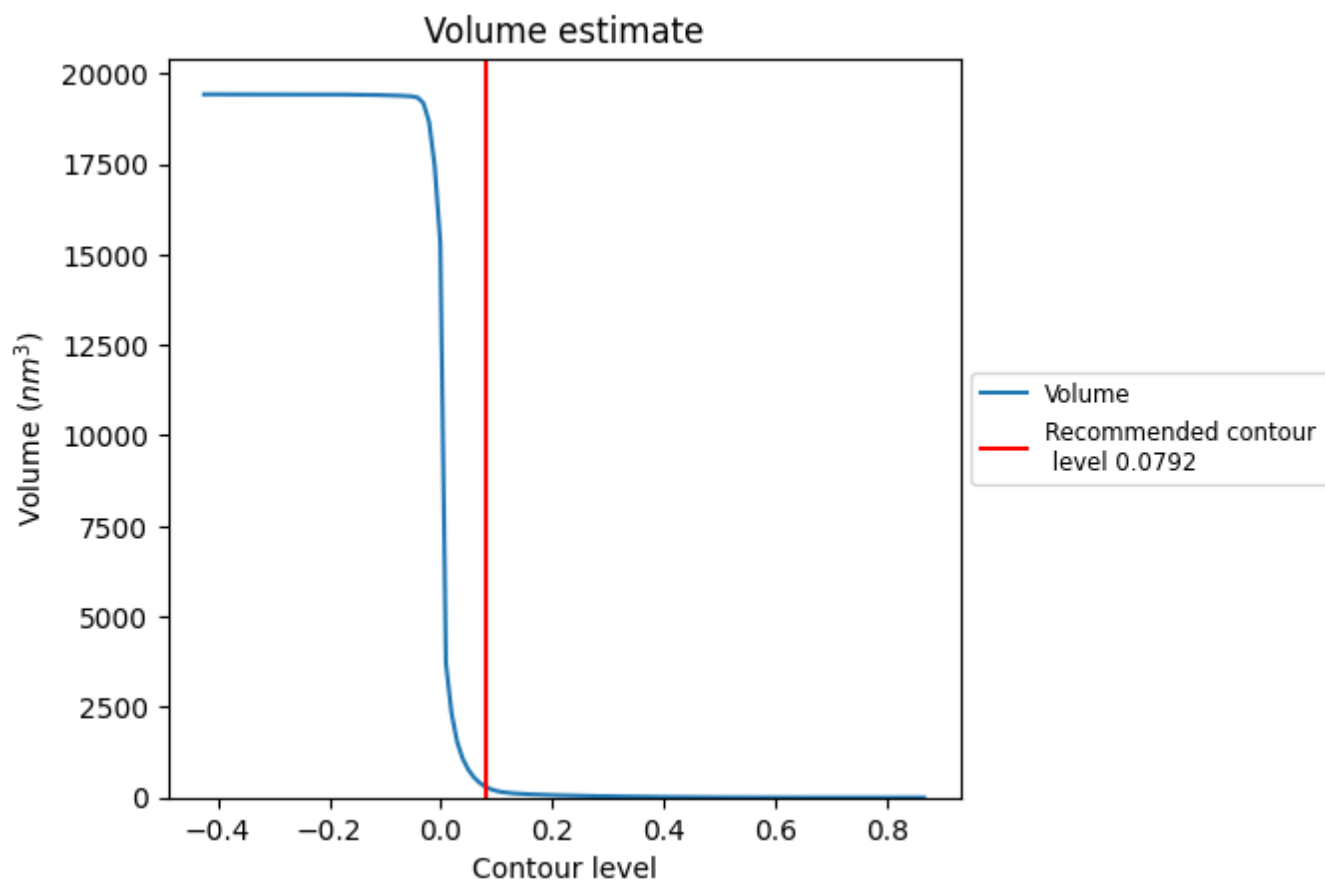
This section contains the results of statistical analysis of the map.

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.

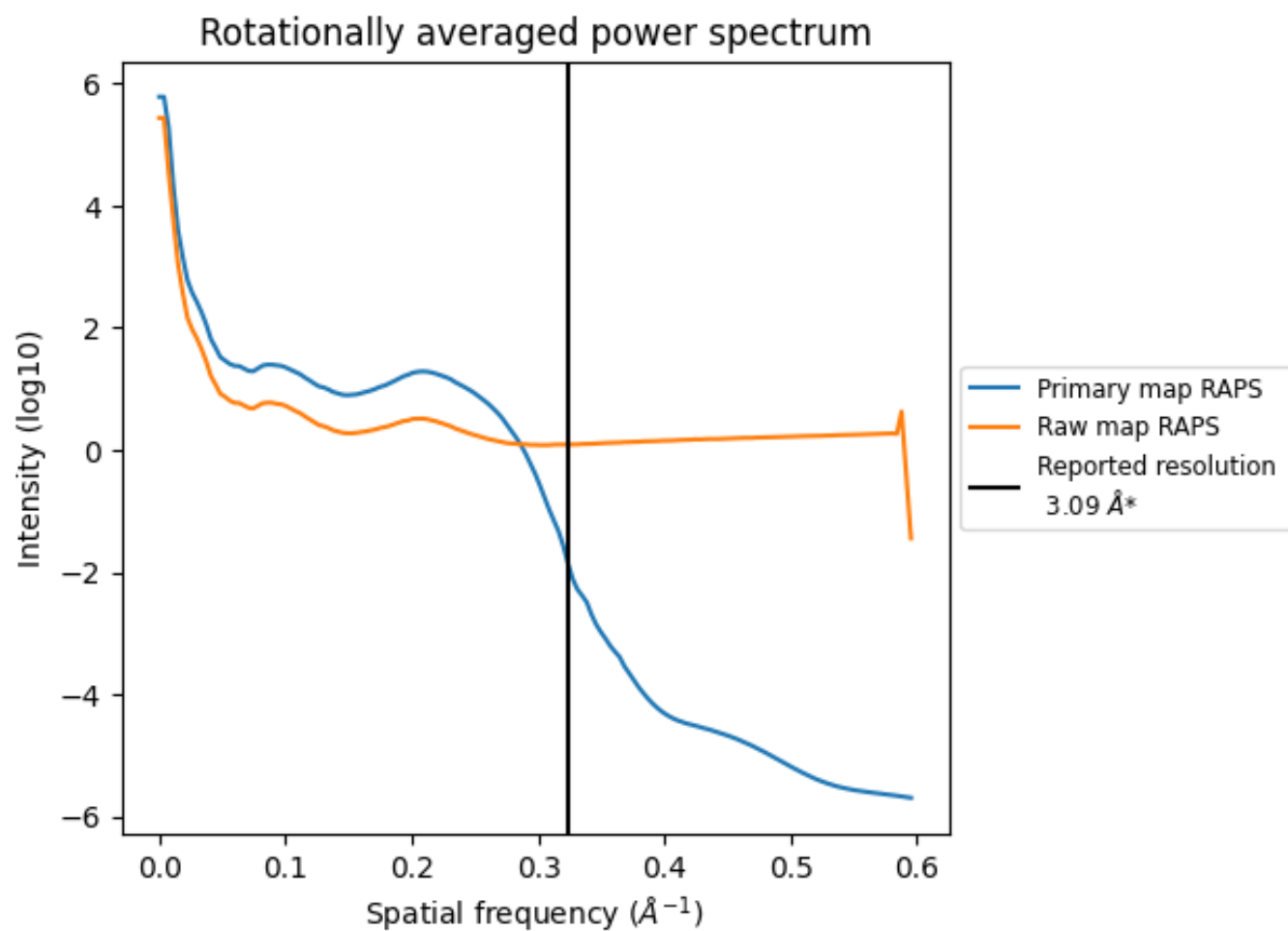
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

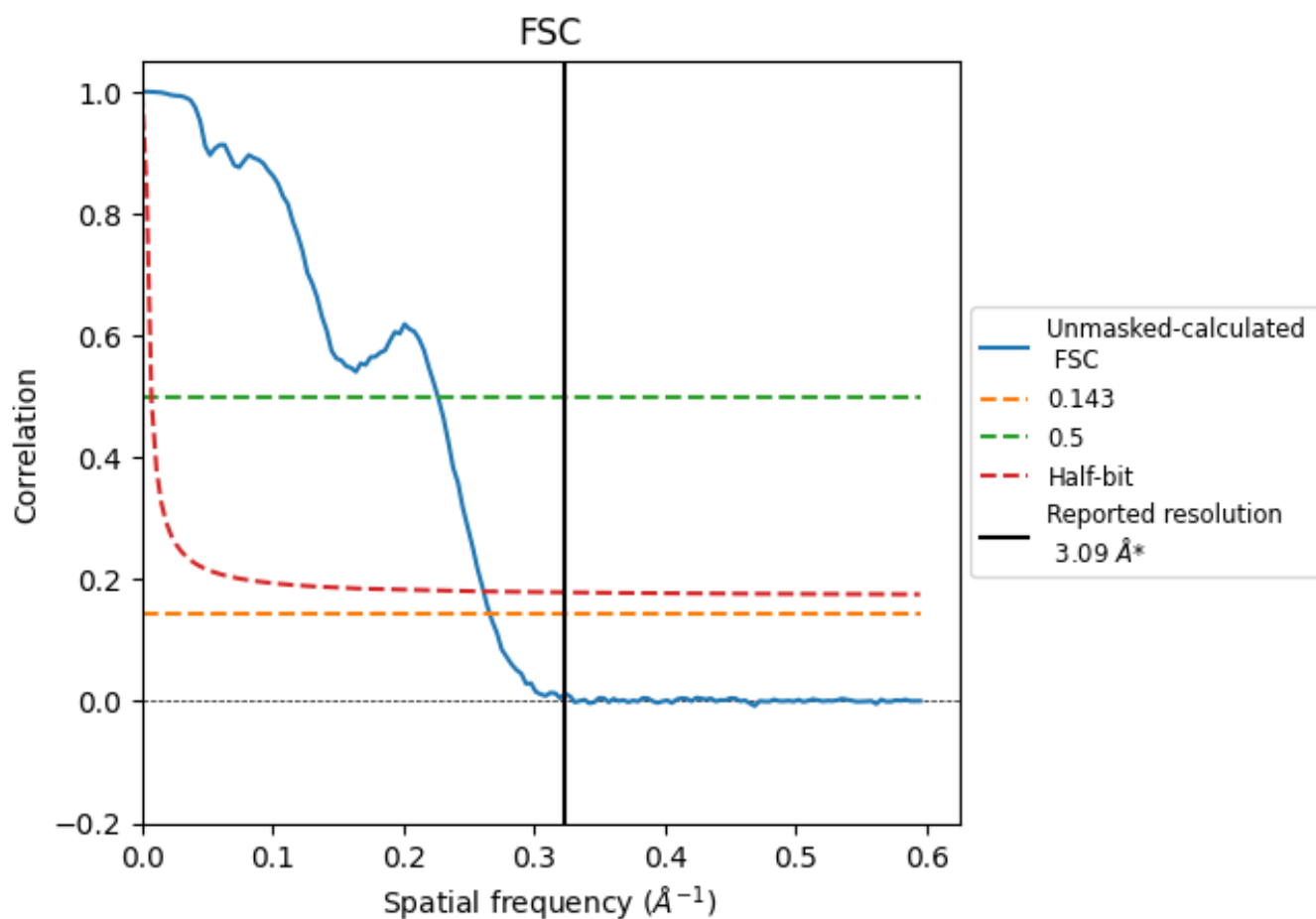


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

8.2 Resolution estimates [i](#)

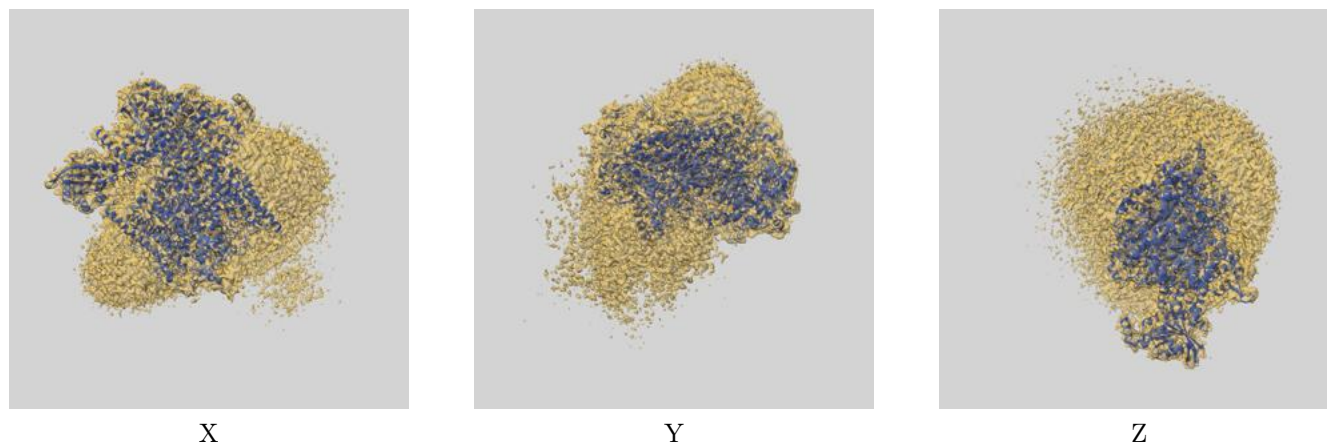
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.42	3.83

*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 3.76 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

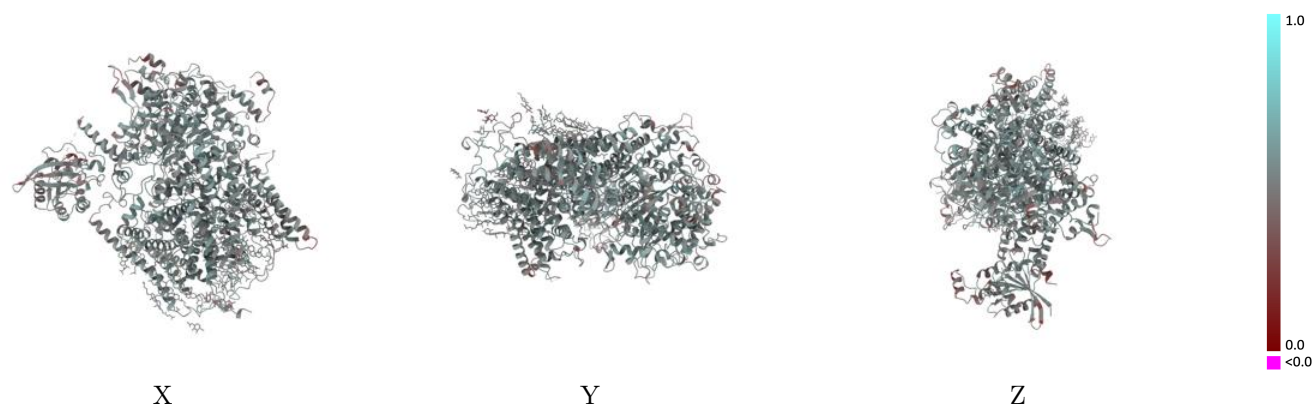
This section contains information regarding the fit between EMDB map EMD-71550 and PDB model 9PE1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



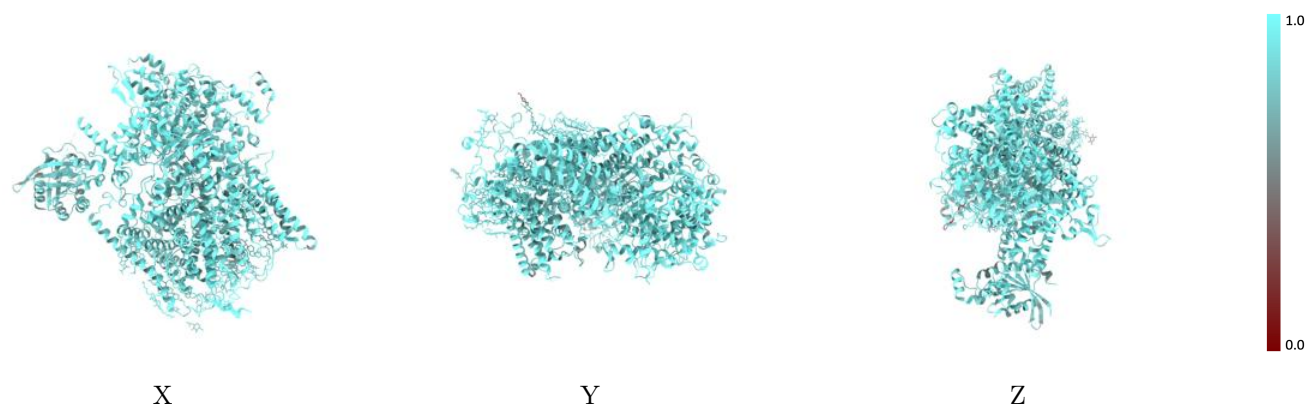
The images above show the 3D surface view of the map at the recommended contour level 0.0792 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



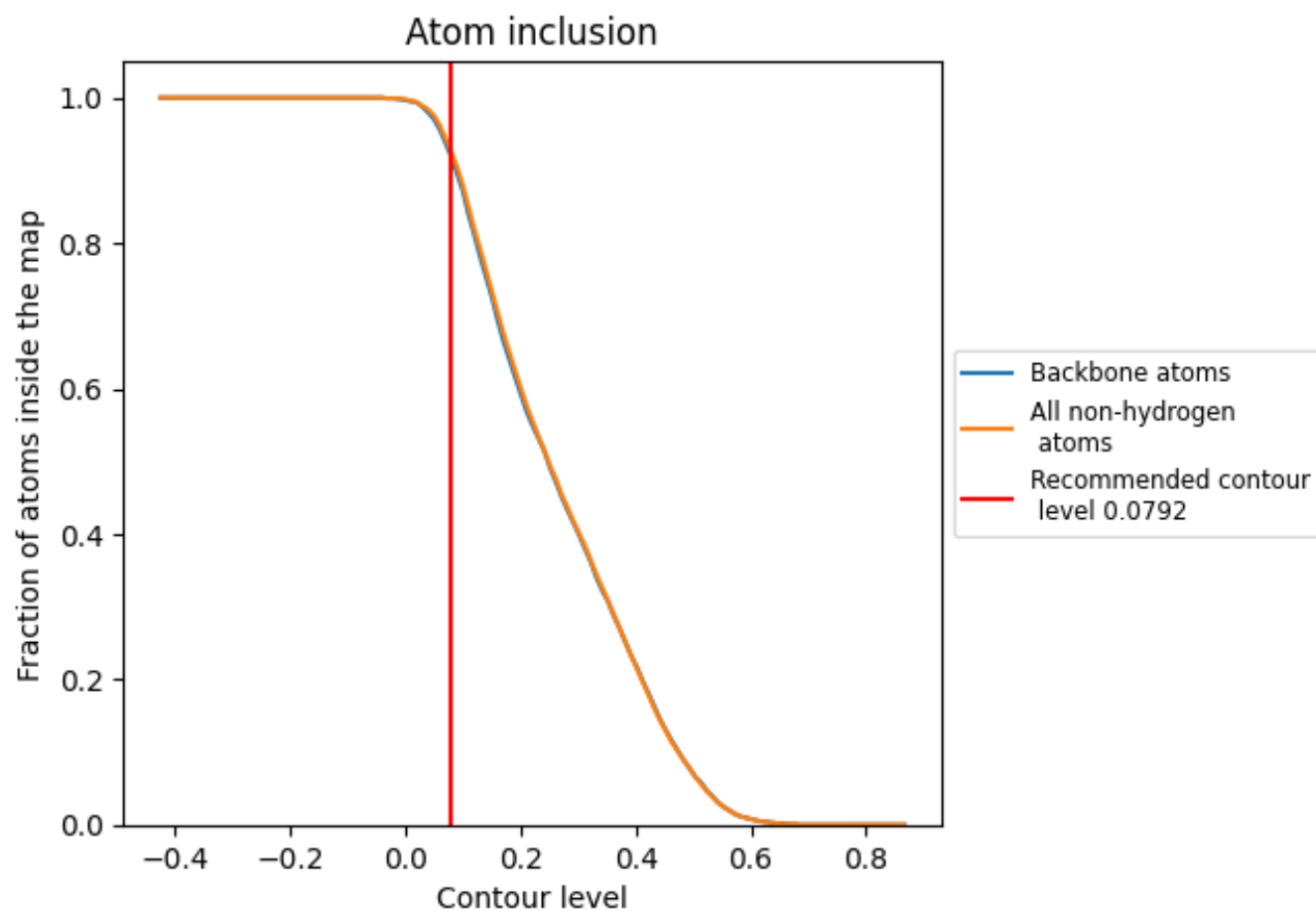
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0792).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (0.0792) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9270	<div><div></div></div> 0.5180
A	<div><div></div></div> 0.9450	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.9150	<div><div></div></div> 0.5280
E	<div><div></div></div> 0.8450	<div><div></div></div> 0.4790
G	<div><div></div></div> 0.8510	<div><div></div></div> 0.4880
H	<div><div></div></div> 0.9550	<div><div></div></div> 0.5060
K	<div><div></div></div> 0.9670	<div><div></div></div> 0.4310

1.0

0.0

<0.0