



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:05 PM UTC

PDB ID : 6BAJ / pdb_00006baj
EMDB ID : EMD-7074
Title : Cryo-EM structure of lipid bilayer in the native cell membrane nanoparticles of AcrB
Authors : Qiu, W.; Fu, Z.; Guo, Y.
Deposited on : 2017-10-13
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

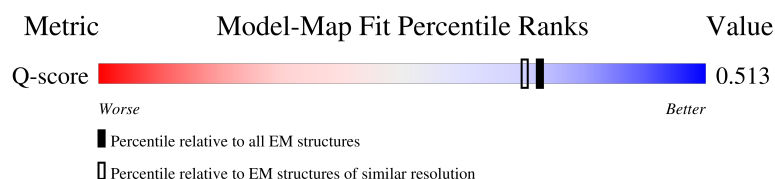
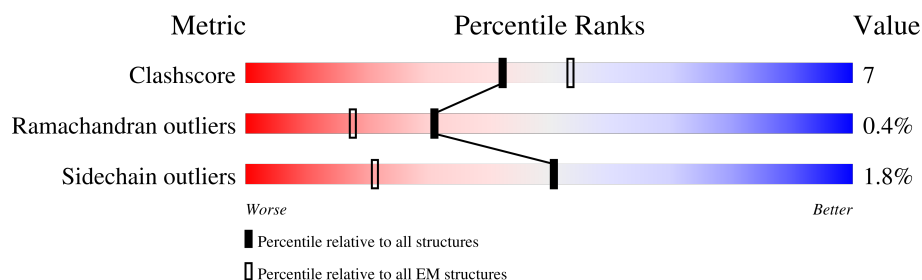
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1057	7% 79% 15% 6%
1	B	1057	81% 15% ..
1	C	1057	85% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24318 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

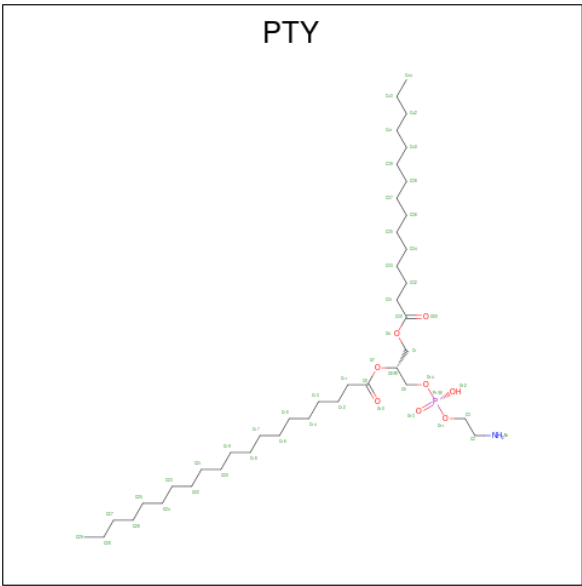
- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1024	Total	C	N	O	S	0	0
			7786	5017	1281	1444	44		
1	C	1023	Total	C	N	O	S	0	0
			7777	5009	1280	1444	44		
1	A	995	Total	C	N	O	S	0	0
			7544	4857	1239	1405	43		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



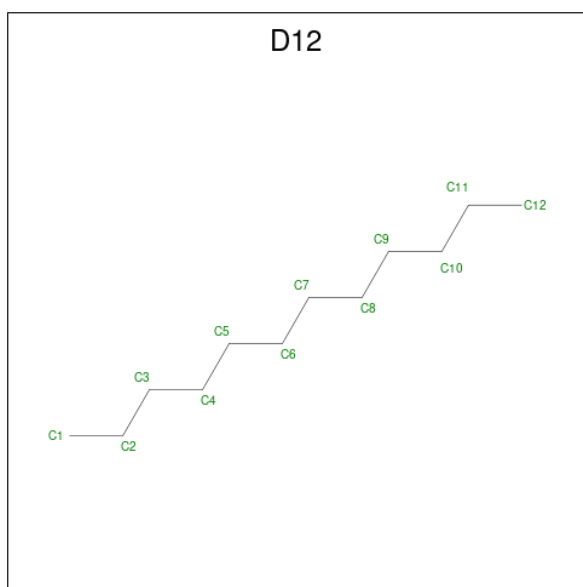
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	B	1	Total	C	N	O	P	0
			29	19	1	8	1	
2	B	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
2	B	1	Total	C	O			0
			28	23	5			
2	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
2	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	C	1	Total	C	N	O	P	0
			22	14	1	6	1	
2	C	1	Total	C	N	O	P	0
			30	20	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C				0
			20	20				
2	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
2	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
2	C	1	Total	C	N	O	P	0
			24	16	1	6	1	
2	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
2	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
2	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
2	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 3 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	C 12 12	0
3	B	1	Total	C 12 12	0
3	B	1	Total	C 9 9	0
3	B	1	Total	C 12 12	0
3	B	1	Total	C 12 12	0
3	B	1	Total	C 12 12	0
3	C	1	Total	C 12 12	0
3	C	1	Total	C 12 12	0
3	C	1	Total	C 12 12	0
3	C	1	Total	C 12 12	0
3	C	1	Total	C 12 12	0

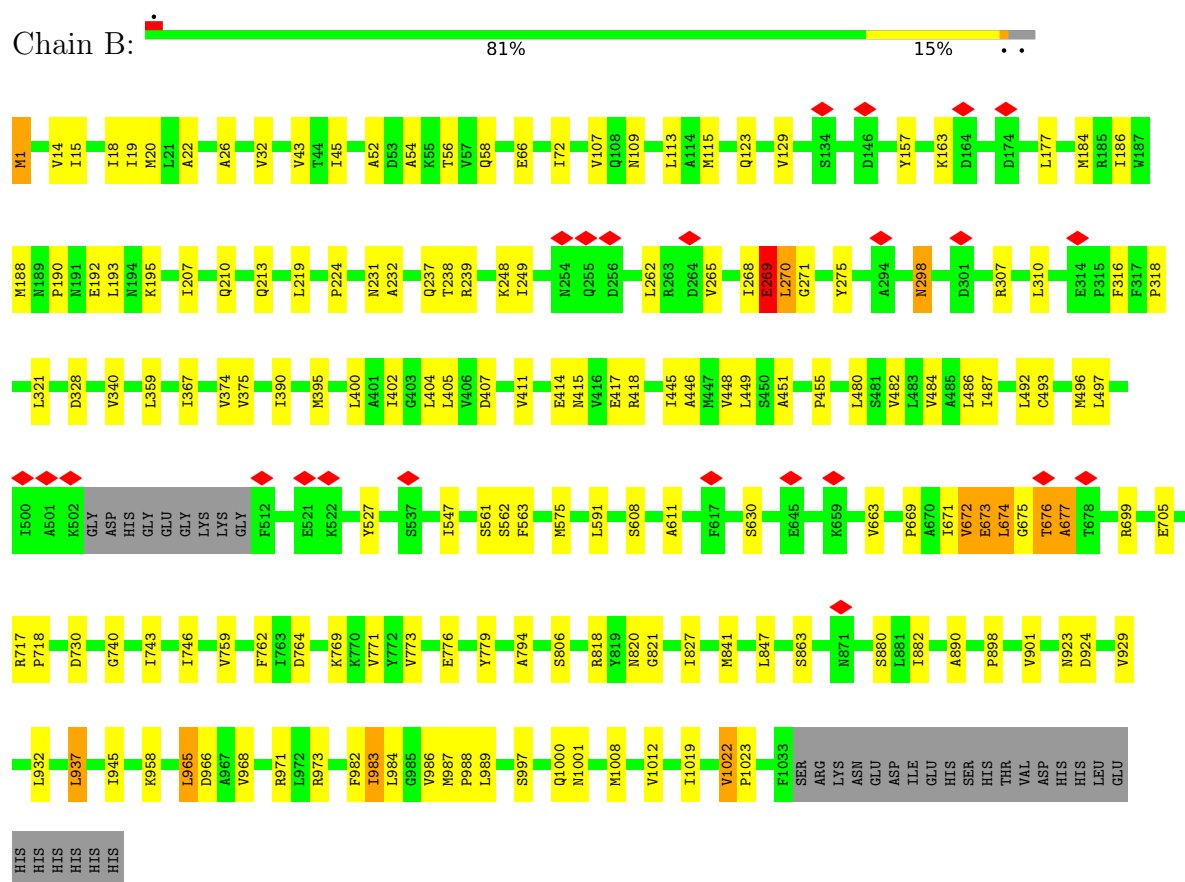
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	O 1 1	0

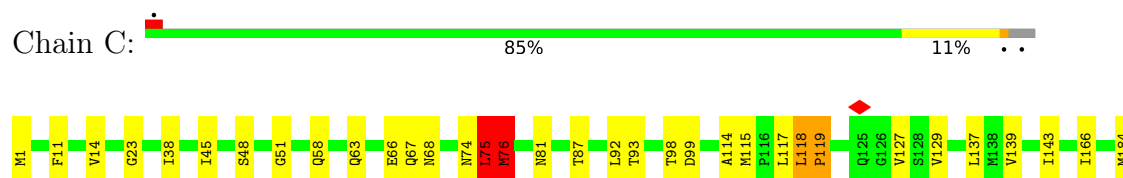
3 Residue-property plots

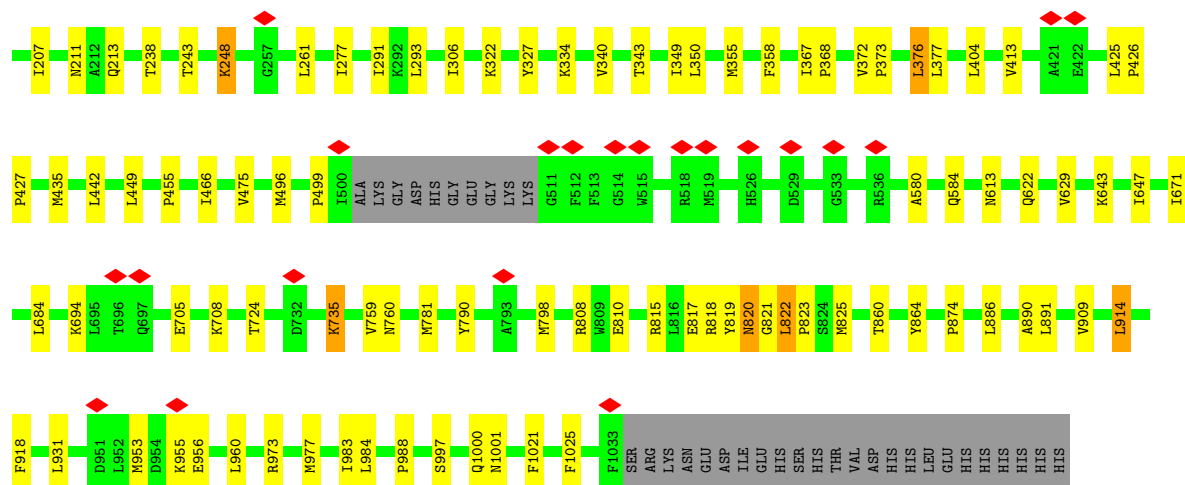
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Multidrug efflux pump subunit AcrB

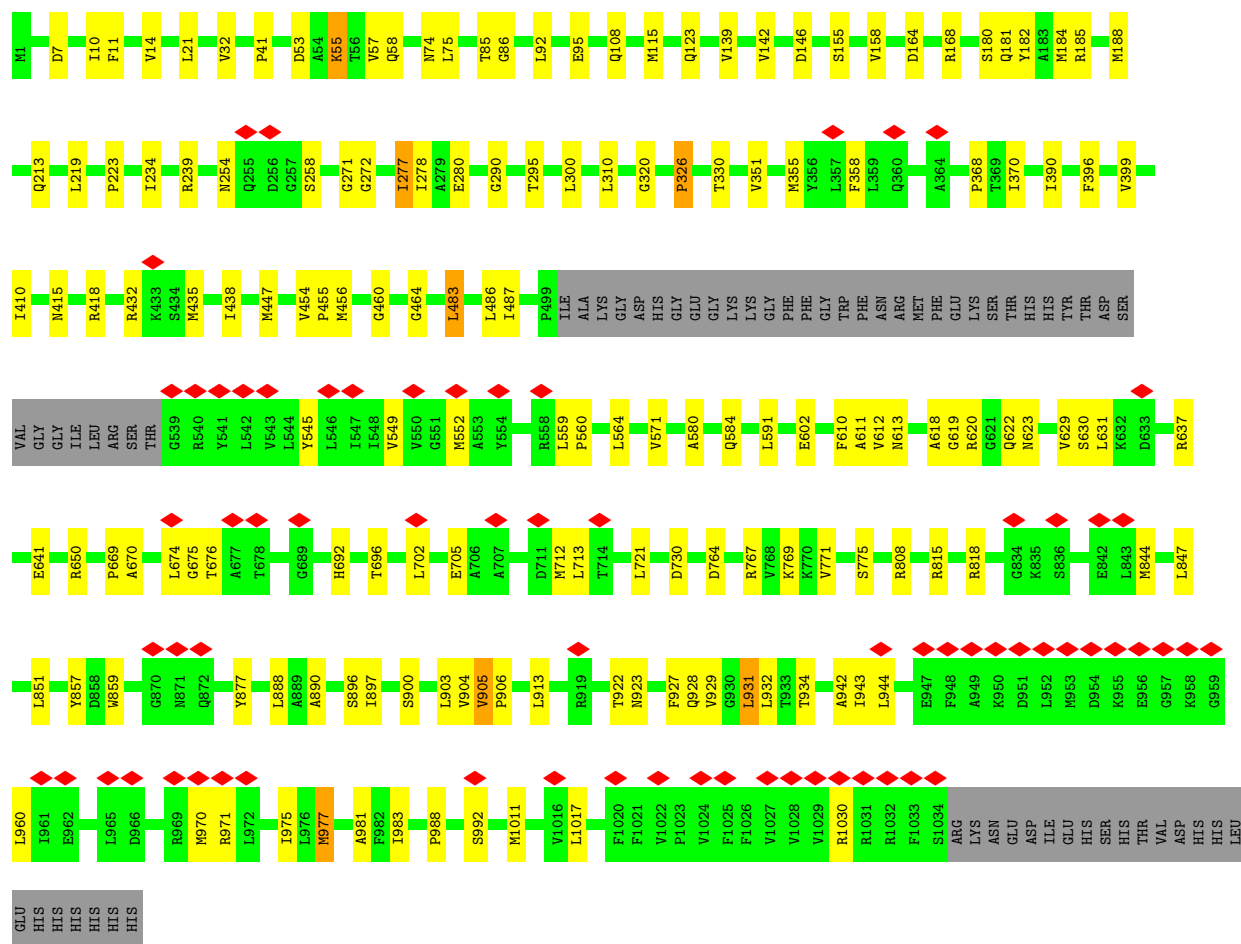
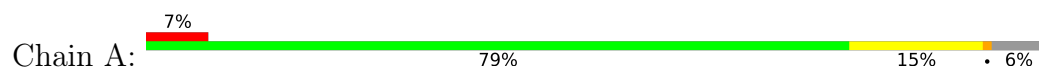


• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.358	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	211.20001, 211.20001, 211.20001	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: D12, PTY

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	0.31	0/7683	0.62	4/10440 (0.0%)
1	B	0.29	0/7934	0.59	0/10777
1	C	0.31	0/7924	0.59	1/10763 (0.0%)
All	All	0.30	0/23541	0.60	5/31980 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	5.61	123.77	120.24
1	A	896	SER	C-N-CA	5.61	123.77	120.24
1	C	75	LEU	N-CA-C	5.37	122.25	110.80
1	A	602	GLU	CA-C-N	5.15	127.44	120.38
1	A	602	GLU	C-N-CA	5.15	127.44	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7544	0	7712	117	0
1	B	7786	0	7940	121	0
1	C	7777	0	7926	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	409	0	539	11	0
2	B	322	0	421	9	0
2	C	350	0	446	14	0
3	B	69	0	147	3	0
3	C	60	0	130	3	0
4	B	1	0	0	0	0
All	All	24318	0	25261	333	0

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

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:SER:HB2	1:B:676:THR:CG2	1.39	1.49
1:A:559:LEU:HD21	1:A:927:PHE:HE2	1.03	1.16
1:B:562:SER:CB	1:B:676:THR:CG2	2.25	1.13
1:B:562:SER:HB2	1:B:676:THR:HG21	1.36	1.06
1:B:676:THR:O	1:B:677:ALA:HB3	1.56	1.04
1:B:562:SER:HB2	1:B:676:THR:HG22	1.36	1.04
1:C:822:LEU:HD12	1:C:823:PRO:HD2	1.39	1.04
1:A:559:LEU:HD21	1:A:927:PHE:CE2	1.93	1.03
1:A:559:LEU:CD2	1:A:927:PHE:HE2	1.73	1.01
1:C:74:ASN:ND2	1:C:98:THR:HG21	1.75	1.00
1:C:74:ASN:HD22	1:C:98:THR:HG21	1.24	0.99
1:B:562:SER:CB	1:B:676:THR:HG22	1.88	0.99
1:A:559:LEU:CD2	1:A:927:PHE:CE2	2.49	0.95
1:B:562:SER:HB2	1:B:676:THR:HG23	1.50	0.89
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.37	0.88
1:C:372:VAL:O	1:C:376:LEU:HD11	1.76	0.86
1:A:913:LEU:HD23	1:A:927:PHE:CZ	2.10	0.85
1:B:676:THR:O	1:B:677:ALA:CB	2.21	0.83
1:A:923:ASN:HB3	1:A:927:PHE:CD2	2.14	0.81
1:B:562:SER:CA	1:B:676:THR:HG22	2.10	0.80
1:C:76:MET:HE2	1:C:864:TYR:HE2	1.47	0.79
1:C:820:ASN:ND2	1:C:820:ASN:O	2.15	0.79
1:C:372:VAL:O	1:C:376:LEU:CG	2.32	0.77
1:A:923:ASN:HA	1:A:927:PHE:HB2	1.70	0.74
1:B:958:LYS:NZ	1:B:966:ASP:OD2	2.20	0.74
1:B:562:SER:HA	1:B:676:THR:HG22	1.68	0.74
1:C:372:VAL:O	1:C:376:LEU:CD1	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:ARG:HH21	1:A:767:ARG:HG3	1.55	0.72
1:A:483:LEU:C	1:A:483:LEU:HD23	2.14	0.72
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.22	0.71
1:B:269:GLU:O	1:B:269:GLU:HG3	1.91	0.70
1:B:818:ARG:NH1	1:B:821:GLY:O	2.25	0.70
1:B:983:ILE:HD12	1:B:1012:VAL:HG22	1.72	0.69
1:C:822:LEU:CD1	1:C:823:PRO:HD2	2.21	0.68
1:A:923:ASN:HA	1:A:927:PHE:CB	2.24	0.67
1:B:268:ILE:O	1:B:269:GLU:O	2.13	0.66
1:C:334:LYS:HZ1	2:C:1104:PTY:HC31	1.59	0.66
1:C:76:MET:HE2	1:C:864:TYR:CE2	2.31	0.66
1:A:631:LEU:HD13	1:A:637:ARG:HH12	1.58	0.66
1:C:815:ARG:NH1	1:C:817:GLU:OE2	2.30	0.65
1:C:694:LYS:HZ1	1:C:825:MET:HG3	1.60	0.65
1:B:983:ILE:O	1:B:983:ILE:HG13	1.97	0.64
1:A:944:LEU:HD12	1:A:971:ARG:HH11	1.63	0.63
1:B:455:PRO:HG2	1:B:880:SER:HB2	1.81	0.62
1:C:372:VAL:O	1:C:376:LEU:HG	2.00	0.62
1:C:74:ASN:ND2	1:C:98:THR:CG2	2.59	0.62
1:A:181:GLN:NE2	1:A:767:ARG:HE	1.97	0.62
1:A:923:ASN:CB	1:A:927:PHE:HB3	2.30	0.62
1:A:631:LEU:HD13	1:A:637:ARG:NH1	2.14	0.61
1:B:207:ILE:HD12	1:B:759:VAL:HG11	1.83	0.61
1:B:562:SER:CB	1:B:676:THR:HG21	2.12	0.60
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.82	0.60
1:A:74:ASN:ND2	1:A:95:GLU:OE2	2.34	0.60
1:C:372:VAL:O	1:C:376:LEU:HD21	2.01	0.60
1:B:672:VAL:O	1:B:672:VAL:HG13	2.02	0.60
1:A:483:LEU:HD11	2:A:1103:PTY:H202	1.83	0.60
1:A:564:LEU:HD23	1:A:670:ALA:HB1	1.85	0.59
1:A:730:ASP:OD2	1:A:808:ARG:NH1	2.34	0.59
1:A:115:MET:O	1:A:123:GLN:NE2	2.35	0.59
1:A:913:LEU:CD2	1:A:927:PHE:CZ	2.82	0.59
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.85	0.59
1:B:414:GLU:OE2	1:B:973:ARG:NE	2.36	0.59
1:C:705:GLU:CD	1:C:708:LYS:HZ1	2.11	0.59
1:B:390:ILE:HG23	1:B:395:MET:HE3	1.86	0.58
1:A:155:SER:HB3	1:A:180:SER:H	1.69	0.58
1:C:143:ILE:HD11	1:C:322:LYS:NZ	2.19	0.58
1:B:66:GLU:OE2	1:B:818:ARG:NE	2.29	0.58
1:B:54:ALA:O	1:B:58:GLN:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HA	1:C:261:LEU:HD23	1.85	0.57
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.86	0.57
1:C:75:LEU:O	1:C:93:THR:O	2.22	0.57
1:B:407:ASP:OD2	1:B:937:LEU:HD21	2.05	0.57
1:B:210:GLN:HG3	1:B:249:ILE:HG12	1.87	0.57
1:A:857:TYR:OH	1:A:859:TRP:NE1	2.38	0.56
1:B:982:PHE:C	1:B:984:LEU:H	2.12	0.56
1:B:192:GLU:HA	1:B:195:LYS:HG2	1.88	0.56
1:C:404:LEU:HD22	1:C:449:LEU:HD21	1.87	0.56
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.87	0.56
1:B:493:CYS:HA	1:B:497:LEU:HD13	1.87	0.56
1:C:184:MET:HE1	1:C:243:THR:HG22	1.88	0.56
1:B:367:ILE:HD12	1:B:492:LEU:HB3	1.87	0.56
1:C:874:PRO:HB3	2:C:1106:PTY:H121	1.87	0.56
1:C:955:LYS:HG3	1:C:956:GLU:HG3	1.88	0.56
2:B:1109:PTY:H171	2:B:1109:PTY:H431	1.88	0.55
1:A:591:LEU:HD12	1:A:611:ALA:HB1	1.87	0.55
2:A:1111:PTY:H111	2:A:1111:PTY:H322	1.87	0.55
1:C:819:TYR:OH	1:C:860:THR:OG1	2.24	0.55
1:B:375:VAL:HG22	1:B:484:VAL:HG11	1.87	0.55
1:B:673:GLU:O	1:B:673:GLU:HG3	2.06	0.55
1:C:358:PHE:O	1:C:973:ARG:NH2	2.39	0.55
1:C:372:VAL:O	1:C:376:LEU:CD2	2.55	0.55
1:A:142:VAL:HG21	1:A:158:VAL:HG21	1.89	0.55
1:B:411:VAL:HG22	1:B:971:ARG:HH22	1.72	0.55
1:B:15:ILE:HA	1:B:18:ILE:HG12	1.89	0.55
1:A:944:LEU:HD12	1:A:971:ARG:NH1	2.21	0.55
1:B:986:VAL:HG23	1:B:1008:MET:CE	2.36	0.55
1:B:15:ILE:HD11	1:B:487:ILE:HG21	1.89	0.54
1:B:19:ILE:HG13	2:B:1107:PTY:H431	1.90	0.54
1:C:66:GLU:OE2	1:C:821:GLY:N	2.40	0.54
1:C:211:ASN:HB3	1:C:760:ASN:HD21	1.72	0.54
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.88	0.54
1:B:986:VAL:HG23	1:B:1008:MET:HE2	1.88	0.54
1:C:213:GLN:HE22	1:C:238:THR:HG22	1.73	0.54
1:A:139:VAL:HG23	1:A:326:PRO:HG2	1.89	0.54
1:A:396:PHE:HA	1:A:399:VAL:HG12	1.90	0.54
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.90	0.54
1:B:298:ASN:OD1	1:B:298:ASN:N	2.38	0.54
1:A:560:PRO:O	1:A:922:THR:OG1	2.26	0.54
2:C:1106:PTY:H341	2:C:1106:PTY:H111	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB2	2:C:1101:PTY:HC6	1.89	0.53
1:C:355:MET:HE3	1:C:368:PRO:HG2	1.89	0.53
1:B:184:MET:HA	1:B:270:LEU:HD23	1.90	0.53
1:C:68:ASN:HD22	1:C:114:ALA:HB2	1.74	0.53
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.91	0.52
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.92	0.52
1:A:435:MET:HE1	1:A:486:LEU:HD23	1.91	0.52
1:A:931:LEU:O	1:A:934:THR:HG22	2.09	0.52
1:C:143:ILE:HD11	1:C:322:LYS:HZ3	1.75	0.52
1:C:340:VAL:HG22	1:C:1000:GLN:HE21	1.75	0.52
1:A:641:GLU:O	1:A:650:ARG:NH2	2.43	0.52
1:A:944:LEU:HB2	1:A:971:ARG:HH11	1.75	0.52
1:A:767:ARG:HH21	1:A:767:ARG:CG	2.17	0.52
1:B:987:MET:N	1:B:988:PRO:CD	2.73	0.52
2:C:1101:PTY:H112	2:A:1102:PTY:H132	1.91	0.51
1:B:359:LEU:HD22	1:B:417:GLU:HG2	1.92	0.51
1:B:157:TYR:OH	1:B:316:PHE:O	2.27	0.51
1:B:676:THR:O	1:B:676:THR:HG22	2.11	0.51
1:A:58:GLN:NE2	1:A:818:ARG:HH11	2.09	0.51
1:B:113:LEU:HD21	1:A:108:GLN:HE22	1.76	0.51
1:B:730:ASP:OD1	1:B:806:SER:OG	2.29	0.51
1:B:318:PRO:HD2	1:B:321:LEU:HD13	1.92	0.51
1:B:776:GLU:HB2	1:B:779:TYR:HD2	1.76	0.51
1:B:26:ALA:HB2	2:B:1106:PTY:H121	1.93	0.51
1:A:21:LEU:HD11	2:A:1101:PTY:H192	1.92	0.51
2:B:1106:PTY:H172	2:B:1107:PTY:H422	1.93	0.51
1:C:997:SER:O	1:C:1001:ASN:ND2	2.45	0.51
1:A:905:VAL:HG13	1:A:906:PRO:HD3	1.92	0.51
1:B:237:GLN:NE2	1:B:238:THR:O	2.44	0.50
1:B:699:ARG:HG3	1:B:827:ILE:HD11	1.92	0.50
1:B:231:ASN:ND2	1:C:622:GLN:OE1	2.45	0.50
1:A:460:GLY:HA2	1:A:464:GLY:HA3	1.92	0.50
1:B:56:THR:HG23	1:A:213:GLN:HG3	1.94	0.50
1:B:898:PRO:HA	1:B:901:VAL:HG22	1.93	0.50
2:B:1108:PTY:H362	2:A:1111:PTY:H361	1.93	0.50
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.94	0.50
1:A:705:GLU:HB3	1:A:847:LEU:HD11	1.94	0.50
1:A:277:ILE:HA	1:A:613:ASN:O	2.11	0.50
1:A:923:ASN:HB3	1:A:927:PHE:HD2	1.74	0.50
1:A:74:ASN:HB3	1:A:95:GLU:HG2	1.94	0.50
1:B:890:ALA:HB1	1:A:11:PHE:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:HD23	1:B:937:LEU:HD23	1.93	0.49
1:B:563:PHE:H	1:B:676:THR:HG23	1.77	0.49
1:A:139:VAL:HG12	1:A:290:GLY:HA2	1.93	0.49
1:A:278:ILE:HG22	1:A:613:ASN:HB3	1.93	0.49
1:A:280:GLU:O	1:A:610:PHE:HA	2.12	0.49
3:C:1113:D12:H81	3:C:1116:D12:H71	1.93	0.49
1:A:355:MET:HE1	1:A:368:PRO:HG2	1.94	0.49
1:B:115:MET:O	1:B:123:GLN:NE2	2.44	0.49
1:B:445:ILE:HG23	1:B:449:LEU:HD12	1.95	0.49
1:C:166:ILE:HD12	1:C:306:ILE:HG23	1.95	0.49
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.95	0.49
1:C:63:GLN:O	1:C:67:GLN:HB2	2.13	0.49
1:A:7:ASP:OD1	1:A:432:ARG:NH2	2.45	0.49
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.94	0.48
1:A:85:THR:HG21	1:A:620:ARG:HH12	1.78	0.48
1:A:545:TYR:OH	1:A:903:LEU:O	2.29	0.48
1:B:415:ASN:OD1	1:B:418:ARG:NH2	2.46	0.48
1:B:22:ALA:HB2	2:C:1102:PTY:H202	1.94	0.48
1:B:402:ILE:HA	1:B:405:LEU:HB2	1.95	0.48
1:B:890:ALA:HB2	1:A:14:VAL:HG11	1.95	0.48
2:C:1102:PTY:H212	2:C:1102:PTY:H331	1.96	0.48
1:B:924:ASP:OD1	1:B:924:ASP:N	2.46	0.48
1:C:886:LEU:HD11	2:C:1103:PTY:H162	1.95	0.48
1:A:674:LEU:HB3	1:A:676:THR:HG23	1.95	0.48
1:A:53:ASP:OD1	1:A:53:ASP:N	2.46	0.48
1:A:185:ARG:NH2	1:A:272:GLY:O	2.47	0.48
1:B:561:SER:HA	1:B:923:ASN:HB3	1.94	0.47
1:A:58:GLN:HE21	1:A:818:ARG:HH11	1.62	0.47
3:C:1113:D12:H61	3:C:1116:D12:H52	1.97	0.47
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.96	0.47
1:C:425:LEU:HD13	1:C:426:PRO:HD2	1.96	0.47
1:A:418:ARG:NH1	1:A:970:MET:HE3	2.30	0.47
1:B:239:ARG:HD3	1:B:762:PHE:HA	1.95	0.47
2:C:1101:PTY:H332	2:C:1110:PTY:H151	1.97	0.47
1:A:619:GLY:HA3	1:A:815:ARG:NH1	2.29	0.47
1:B:270:LEU:HD22	1:B:271:GLY:H	1.79	0.47
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.95	0.47
2:B:1105:PTY:H132	2:A:1108:PTY:H151	1.96	0.47
1:C:277:ILE:HA	1:C:613:ASN:O	2.14	0.47
1:C:808:ARG:NH2	1:C:810:GLU:OE2	2.48	0.47
2:C:1110:PTY:H112	2:C:1110:PTY:H141	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HG2	1:A:775:SER:HA	1.97	0.47
1:C:115:MET:HE1	1:C:127:VAL:HB	1.96	0.47
1:A:415:ASN:HD22	1:A:438:ILE:HG12	1.79	0.47
1:A:454:VAL:HG23	1:A:455:PRO:HD3	1.97	0.46
1:B:527:TYR:OH	1:B:1019:ILE:O	2.32	0.46
1:B:562:SER:HA	1:B:676:THR:O	2.14	0.46
1:C:14:VAL:HG11	1:A:890:ALA:HB2	1.97	0.46
2:C:1110:PTY:H162	1:A:447:MET:HE3	1.98	0.46
1:A:619:GLY:HA3	1:A:815:ARG:HH12	1.80	0.46
1:B:72:ILE:HD13	1:B:107:VAL:HG22	1.98	0.46
1:C:207:ILE:HG13	1:C:759:VAL:HG11	1.96	0.46
1:A:55:LYS:HD3	1:A:55:LYS:HA	1.70	0.46
1:C:350:LEU:HD12	1:C:984:LEU:HD23	1.97	0.46
1:C:983:ILE:HG13	1:C:984:LEU:HD12	1.96	0.46
1:B:965:LEU:HA	1:B:968:VAL:HG12	1.97	0.46
2:B:1104:PTY:HC12	2:A:1103:PTY:H311	1.97	0.46
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.98	0.46
1:A:767:ARG:HG3	1:A:767:ARG:NH2	2.28	0.46
1:A:456:MET:HE3	1:A:932:LEU:HD22	1.97	0.46
2:B:1101:PTY:H132	1:C:891:LEU:HD23	1.98	0.46
1:A:85:THR:HG21	1:A:620:ARG:NH1	2.31	0.46
1:A:944:LEU:HG	1:A:971:ARG:HE	1.80	0.46
1:C:694:LYS:NZ	1:C:825:MET:HG3	2.29	0.46
1:B:764:ASP:HB3	1:B:769:LYS:HD3	1.97	0.46
1:C:38:ILE:HD11	1:C:671:ILE:HG21	1.97	0.46
1:C:372:VAL:HG23	1:C:373:PRO:HD3	1.98	0.45
1:B:20:MET:HB2	1:B:374:VAL:HG23	1.98	0.45
1:B:989:LEU:HG	1:B:1000:GLN:HB3	1.98	0.45
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.99	0.45
1:A:877:TYR:OH	1:A:928:GLN:HG2	2.15	0.45
1:B:270:LEU:HD22	1:B:271:GLY:N	2.30	0.45
1:C:435:MET:HE3	1:C:435:MET:HB3	1.78	0.45
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.99	0.45
1:A:983:ILE:HD11	1:A:1011:MET:HB3	1.98	0.45
1:C:953:MET:HE2	1:C:960:LEU:HA	1.99	0.45
1:A:584:GLN:HB2	1:A:622:GLN:HE21	1.82	0.45
1:C:367:ILE:HD11	1:C:496:MET:HB2	1.98	0.45
1:C:790:TYR:HB3	1:C:798:MET:HB2	1.97	0.45
1:B:1:MET:HE2	1:B:487:ILE:HD11	1.99	0.45
1:B:32:VAL:H	1:B:298:ASN:HB3	1.81	0.45
1:C:75:LEU:HD21	1:C:92:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:MET:SD	1:A:712:MET:N	2.89	0.44
1:A:767:ARG:CG	1:A:767:ARG:NH2	2.73	0.44
1:A:927:PHE:O	1:A:927:PHE:CD1	2.70	0.44
1:B:496:MET:HE2	3:B:1114:D12:H91	1.98	0.44
1:C:207:ILE:HD11	1:C:759:VAL:HG21	1.99	0.44
1:A:75:LEU:HD11	1:A:92:LEU:HD23	1.99	0.44
1:B:213:GLN:NE2	1:C:51:GLY:O	2.47	0.44
1:B:675:GLY:O	1:B:676:THR:C	2.59	0.44
1:A:669:PRO:HD3	1:A:675:GLY:HA2	1.98	0.44
1:B:186:ILE:HB	1:B:773:VAL:HG12	1.98	0.44
1:B:52:ALA:HB1	1:B:56:THR:HB	2.00	0.44
1:C:11:PHE:HD1	1:A:890:ALA:HB1	1.82	0.44
2:C:1102:PTY:H342	2:C:1102:PTY:H171	1.98	0.44
1:A:32:VAL:HG22	1:A:390:ILE:HD11	1.99	0.44
1:B:740:GLY:O	1:B:794:ALA:N	2.50	0.44
1:A:11:PHE:HE1	2:A:1104:PTY:H352	1.83	0.44
1:A:904:VAL:HG11	1:A:942:ALA:HB2	1.99	0.44
1:C:643:LYS:O	1:C:647:ILE:HD12	2.17	0.44
1:A:960:LEU:HD21	1:A:1030:ARG:HG3	2.00	0.43
1:B:163:LYS:NZ	1:B:177:LEU:HB2	2.33	0.43
1:A:219:LEU:HB3	1:A:234:ILE:HD11	1.99	0.43
1:B:219:LEU:N	1:B:232:ALA:O	2.52	0.43
1:C:137:LEU:HD22	1:C:293:LEU:HD13	2.00	0.43
1:A:549:VAL:O	1:A:552:MET:HB3	2.18	0.43
1:C:81:ASN:HD22	1:C:815:ARG:HH21	1.66	0.43
1:B:608:SER:OG	1:B:630:SER:OG	2.37	0.43
1:A:988:PRO:O	1:A:992:SER:OG	2.33	0.43
1:B:58:GLN:HE21	1:B:818:ARG:HD2	1.83	0.43
1:C:45:ILE:HG12	1:C:129:VAL:HG22	2.01	0.43
1:C:798:MET:N	1:C:798:MET:SD	2.91	0.43
1:A:713:LEU:HD21	1:A:844:MET:HG2	2.01	0.43
1:C:48:SER:HA	1:C:87:THR:HA	2.00	0.43
1:C:914:LEU:HD11	1:C:918:PHE:CE2	2.54	0.43
1:A:580:ALA:HA	1:A:623:ASN:HD22	1.84	0.43
1:A:721:LEU:HD12	1:A:815:ARG:HB2	2.00	0.43
1:C:99:ASP:OD1	1:C:99:ASP:N	2.52	0.43
1:B:249:ILE:HB	1:B:262:LEU:HD13	2.01	0.43
1:B:997:SER:O	1:B:1001:ASN:ND2	2.52	0.43
1:A:358:PHE:HD2	1:A:977:MET:HB3	1.83	0.43
1:B:945:ILE:HD11	1:B:1022:VAL:HB	2.01	0.42
1:A:10:ILE:HD11	2:A:1101:PTY:HC21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ASN:HB3	1:A:927:PHE:CG	2.53	0.42
2:A:1111:PTY:H212	2:A:1111:PTY:H242	1.80	0.42
1:B:449:LEU:C	1:B:451:ALA:N	2.76	0.42
1:C:475:VAL:HG11	2:C:1111:PTY:H312	2.01	0.42
1:A:181:GLN:HE22	1:A:767:ARG:HE	1.65	0.42
1:B:188:MET:HE3	1:B:773:VAL:HB	2.00	0.42
1:C:822:LEU:HD13	1:C:822:LEU:HA	1.81	0.42
1:A:182:TYR:HA	1:A:271:GLY:O	2.19	0.42
1:B:224:PRO:HA	1:C:781:MET:HE1	2.02	0.42
1:A:618:ALA:O	1:A:815:ARG:NH2	2.52	0.42
1:A:351:VAL:HG23	1:A:981:ALA:HB1	2.01	0.42
1:B:268:ILE:O	1:B:269:GLU:C	2.62	0.42
1:B:987:MET:CB	1:B:988:PRO:HD3	2.50	0.42
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.02	0.42
1:C:376:LEU:HG	1:C:376:LEU:H	1.58	0.42
1:A:692:HIS:O	1:A:696:THR:OG1	2.31	0.42
1:C:735:LYS:HD2	1:C:735:LYS:HA	1.45	0.42
1:C:1021:PHE:HB3	1:C:1025:PHE:CE2	2.55	0.42
1:A:57:VAL:HG21	1:A:86:GLY:HA2	2.02	0.42
1:B:193:LEU:HD22	1:B:265:VAL:HB	2.02	0.42
3:C:1114:D12:H13	3:C:1116:D12:H13	2.02	0.42
1:A:254:ASN:HB2	1:A:258:SER:HB3	2.02	0.42
1:A:571:VAL:HG23	1:A:630:SER:HA	2.01	0.42
1:C:11:PHE:CD1	1:A:890:ALA:HB1	2.55	0.42
1:B:671:ILE:HG23	1:B:672:VAL:H	1.85	0.41
1:B:983:ILE:HD12	1:B:1012:VAL:CG2	2.45	0.41
1:C:427:PRO:HD3	1:C:499:PRO:HG3	2.01	0.41
2:C:1101:PTY:H311	2:C:1110:PTY:H131	2.02	0.41
1:B:445:ILE:HA	1:B:448:VAL:HG12	2.02	0.41
1:B:717:ARG:HA	1:B:718:PRO:HD3	1.94	0.41
1:A:164:ASP:OD2	1:A:767:ARG:NH1	2.53	0.41
1:A:213:GLN:HB2	1:A:239:ARG:HG3	2.02	0.41
1:B:109:ASN:HB3	1:A:108:GLN:HG2	2.02	0.41
1:B:841:MET:SD	1:B:863:SER:OG	2.67	0.41
1:C:909:VAL:HG13	1:C:931:LEU:HD11	2.02	0.41
1:C:118:LEU:HA	1:C:119:PRO:HD3	1.88	0.41
1:A:146:ASP:OD2	1:A:320:GLY:HA3	2.20	0.41
2:B:1106:PTY:H281	2:B:1106:PTY:H251	1.94	0.41
3:B:1110:D12:H122	3:B:1114:D12:H42	2.02	0.41
1:A:41:PRO:HB3	1:A:295:THR:HG21	2.03	0.41
1:B:43:VAL:HG11	1:B:107:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ILE:CD1	1:B:1012:VAL:HG22	2.46	0.41
1:A:897:ILE:O	1:A:900:SER:OG	2.34	0.41
1:B:190:PRO:HA	1:B:193:LEU:HB2	2.03	0.41
1:B:705:GLU:HB3	1:B:847:LEU:HD11	2.03	0.41
1:B:820:ASN:O	1:A:168:ARG:NH2	2.54	0.41
1:C:58:GLN:HE21	1:C:818:ARG:HD2	1.86	0.41
1:A:58:GLN:HE21	1:A:818:ARG:HD2	1.85	0.41
1:B:496:MET:HG2	3:B:1114:D12:H112	2.02	0.41
1:A:300:LEU:HD23	1:A:330:THR:HG23	2.03	0.41
1:B:400:LEU:HD11	1:B:929:VAL:HG12	2.02	0.40
1:C:368:PRO:HD3	1:C:413:VAL:HG21	2.03	0.40
1:C:584:GLN:HB2	1:C:622:GLN:HE21	1.85	0.40
1:B:19:ILE:HD11	1:B:480:LEU:HD11	2.03	0.40
2:A:1108:PTY:H141	2:A:1108:PTY:H111	1.81	0.40
1:B:575:MET:O	1:B:663:VAL:HA	2.21	0.40
1:A:923:ASN:HA	1:A:927:PHE:HB3	1.99	0.40
1:B:275:TYR:HD2	1:A:223:PRO:HD3	1.87	0.40
1:C:23:GLY:HA3	1:C:377:LEU:O	2.22	0.40
1:C:58:GLN:HE21	1:C:818:ARG:HH21	1.68	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	991/1057 (94%)	920 (93%)	69 (7%)	2 (0%)	43 73
1	B	1020/1057 (96%)	951 (93%)	61 (6%)	8 (1%)	16 50
1	C	1019/1057 (96%)	947 (93%)	69 (7%)	3 (0%)	36 68
All	All	3030/3171 (96%)	2818 (93%)	199 (7%)	13 (0%)	31 62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	673	GLU
1	B	269	GLU
1	B	674	LEU
1	B	677	ALA
1	B	669	PRO
1	B	676	THR
1	C	76	MET
1	B	672	VAL
1	C	75	LEU
1	B	983	ILE
1	A	326	PRO
1	A	929	VAL
1	C	119	PRO

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	809/863 (94%)	795 (98%)	14 (2%)	53	75
1	B	833/863 (96%)	819 (98%)	14 (2%)	53	75
1	C	833/863 (96%)	817 (98%)	16 (2%)	50	73
All	All	2475/2589 (96%)	2431 (98%)	44 (2%)	51	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	248	LYS
1	B	269	GLU
1	B	270	LEU
1	B	298	ASN
1	B	310	LEU
1	B	486	LEU
1	B	547	ILE
1	B	674	LEU
1	B	882	ILE

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Mol	Chain	Res	Type
1	B	932	LEU
1	B	937	LEU
1	B	965	LEU
1	B	1022	VAL
1	C	75	LEU
1	C	76	MET
1	C	117	LEU
1	C	118	LEU
1	C	248	LYS
1	C	349	ILE
1	C	376	LEU
1	C	442	LEU
1	C	455	PRO
1	C	466	ILE
1	C	629	VAL
1	C	684	LEU
1	C	735	LYS
1	C	820	ASN
1	C	822	LEU
1	C	914	LEU
1	A	55	LYS
1	A	277	ILE
1	A	310	LEU
1	A	370	ILE
1	A	410	ILE
1	A	483	LEU
1	A	487	ILE
1	A	612	VAL
1	A	629	VAL
1	A	905	VAL
1	A	931	LEU
1	A	975	ILE
1	A	977	MET
1	A	1017	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	120	GLN
1	B	228	GLN
1	B	231	ASN

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Mol	Chain	Res	Type
1	B	274	ASN
1	B	338	HIS
1	B	526	HIS
1	B	584	GLN
1	B	709	HIS
1	B	871	ASN
1	B	923	ASN
1	B	1001	ASN
1	C	58	GLN
1	C	68	ASN
1	C	74	ASN
1	C	151	GLN
1	C	176	GLN
1	C	181	GLN
1	C	213	GLN
1	C	569	GLN
1	C	701	GLN
1	C	737	GLN
1	C	1000	GLN
1	C	1001	ASN
1	A	58	GLN
1	A	89	GLN
1	A	106	GLN
1	A	181	GLN
1	A	231	ASN
1	A	298	ASN
1	A	360	GLN
1	A	415	ASN
1	A	667	ASN
1	A	692	HIS
1	A	701	GLN
1	A	928	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PTY	A	1111	-	43,43,49	0.94	4 (9%)	46,48,54	1.07	2 (4%)
2	PTY	C	1107	-	30,30,49	1.12	4 (13%)	33,35,54	1.21	2 (6%)
2	PTY	B	1105	-	27,27,49	1.04	4 (14%)	29,29,54	1.19	2 (6%)
2	PTY	B	1106	-	41,41,49	0.96	4 (9%)	44,46,54	1.11	2 (4%)
3	D12	C	1113	-	11,11,11	0.27	0	10,10,10	0.85	0
3	D12	C	1115	-	11,11,11	0.30	0	10,10,10	0.81	0
2	PTY	A	1107	-	31,31,49	1.10	4 (12%)	34,36,54	1.33	2 (5%)
3	D12	C	1114	-	11,11,11	0.27	0	10,10,10	0.89	0
2	PTY	C	1102	-	38,38,49	1.00	4 (10%)	41,43,54	1.18	2 (4%)
2	PTY	B	1103	-	32,32,49	1.08	4 (12%)	35,37,54	1.10	2 (5%)
2	PTY	C	1108	-	33,33,49	1.07	4 (12%)	36,38,54	1.20	2 (5%)
3	D12	B	1115	-	11,11,11	0.30	0	10,10,10	0.80	0
2	PTY	A	1104	-	42,42,49	0.94	4 (9%)	45,47,54	1.15	2 (4%)
2	PTY	B	1108	-	34,34,49	1.04	4 (11%)	37,39,54	1.14	2 (5%)
2	PTY	C	1109	-	35,35,49	1.04	4 (11%)	38,40,54	1.18	2 (5%)
2	PTY	A	1105	-	30,30,49	1.11	4 (13%)	33,35,54	1.14	2 (6%)
2	PTY	A	1108	-	32,32,49	1.08	4 (12%)	35,37,54	1.13	3 (8%)
2	PTY	A	1109	-	37,37,49	1.00	4 (10%)	40,42,54	1.14	3 (7%)
2	PTY	C	1103	-	21,21,49	1.00	1 (4%)	23,24,54	0.97	1 (4%)
2	PTY	B	1107	-	42,42,49	0.95	4 (9%)	45,47,54	1.15	2 (4%)
3	D12	C	1116	-	11,11,11	0.29	0	10,10,10	0.81	0
2	PTY	B	1102	-	28,28,49	1.15	4 (14%)	31,33,54	1.24	2 (6%)
2	PTY	C	1110	-	37,37,49	1.01	4 (10%)	40,42,54	1.12	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PTY	A	1110	-	28,28,49	1.12	3 (10%)	31,33,54	1.21	2 (6%)
2	PTY	C	1111	-	23,23,49	0.93	1 (4%)	25,26,54	0.94	1 (4%)
3	D12	B	1113	-	11,11,11	0.28	0	10,10,10	0.82	0
2	PTY	C	1101	-	31,31,49	1.10	4 (12%)	34,36,54	1.12	2 (5%)
2	PTY	A	1106	-	36,36,49	1.01	4 (11%)	39,41,54	1.13	2 (5%)
3	D12	C	1112	-	11,11,11	0.28	0	10,10,10	0.86	0
2	PTY	A	1101	-	49,49,49	0.89	4 (8%)	52,54,54	1.13	2 (3%)
2	PTY	C	1104	-	29,29,49	1.12	4 (13%)	32,34,54	1.20	2 (6%)
3	D12	B	1110	-	11,11,11	0.26	0	10,10,10	0.87	0
2	PTY	B	1101	-	39,39,49	0.98	4 (10%)	42,44,54	1.12	2 (4%)
2	PTY	A	1102	-	33,33,49	1.05	4 (12%)	36,38,54	1.28	2 (5%)
2	PTY	C	1105	-	19,19,49	0.30	0	18,18,54	0.86	0
2	PTY	B	1109	-	40,40,49	0.97	4 (10%)	43,45,54	1.13	2 (4%)
2	PTY	B	1104	-	30,30,49	1.11	4 (13%)	33,35,54	1.20	2 (6%)
3	D12	B	1112	-	8,8,11	0.27	0	7,7,10	0.81	0
3	D12	B	1114	-	11,11,11	0.30	0	10,10,10	0.78	0
2	PTY	C	1106	-	43,43,49	0.94	4 (9%)	46,48,54	1.09	2 (4%)
2	PTY	A	1103	-	37,37,49	1.01	4 (10%)	40,42,54	1.16	2 (5%)
3	D12	B	1111	-	11,11,11	0.26	0	10,10,10	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	A	1111	-	-	20/47/47/53	-
2	PTY	C	1107	-	-	14/34/34/53	-
2	PTY	B	1105	-	-	10/29/29/53	-
2	PTY	B	1106	-	-	17/45/45/53	-
3	D12	C	1113	-	-	1/9/9/9	-
3	D12	C	1115	-	-	4/9/9/9	-
2	PTY	A	1107	-	-	17/34/34/53	-
3	D12	C	1114	-	-	0/9/9/9	-
2	PTY	C	1102	-	-	12/42/42/53	-
2	PTY	B	1103	-	-	14/36/36/53	-
2	PTY	C	1108	-	-	20/37/37/53	-
3	D12	B	1115	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	A	1104	-	-	19/46/46/53	-
2	PTY	B	1108	-	-	21/38/38/53	-
2	PTY	C	1109	-	-	16/39/39/53	-
2	PTY	A	1105	-	-	12/34/34/53	-
2	PTY	A	1108	-	-	14/36/36/53	-
2	PTY	A	1109	-	-	19/41/41/53	-
2	PTY	C	1103	-	-	10/22/22/53	-
2	PTY	B	1107	-	-	17/46/46/53	-
3	D12	C	1116	-	-	2/9/9/9	-
2	PTY	B	1102	-	-	9/32/32/53	-
2	PTY	C	1110	-	-	14/41/41/53	-
2	PTY	A	1110	-	-	18/32/32/53	-
2	PTY	C	1111	-	-	15/24/24/53	-
3	D12	B	1113	-	-	3/9/9/9	-
2	PTY	C	1101	-	-	14/35/35/53	-
2	PTY	A	1106	-	-	18/40/40/53	-
3	D12	C	1112	-	-	0/9/9/9	-
2	PTY	A	1101	-	-	24/53/53/53	-
2	PTY	C	1104	-	-	20/33/33/53	-
3	D12	B	1110	-	-	4/9/9/9	-
2	PTY	B	1101	-	-	19/43/43/53	-
2	PTY	A	1102	-	-	13/37/37/53	-
2	PTY	C	1105	-	-	5/17/17/53	-
2	PTY	B	1109	-	-	23/44/44/53	-
2	PTY	B	1104	-	-	14/34/34/53	-
3	D12	B	1112	-	-	2/6/6/9	-
3	D12	B	1114	-	-	3/9/9/9	-
2	PTY	C	1106	-	-	18/47/47/53	-
2	PTY	A	1103	-	-	13/41/41/53	-
3	D12	B	1111	-	-	0/9/9/9	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1107	PTY	O7-C6	-2.77	1.40	1.46
2	C	1102	PTY	O7-C6	-2.77	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1107	PTY	O7-C6	-2.77	1.40	1.46
2	A	1105	PTY	O7-C6	-2.76	1.40	1.46
2	A	1106	PTY	O7-C6	-2.76	1.40	1.46
2	A	1108	PTY	O7-C6	-2.74	1.40	1.46
2	A	1109	PTY	O7-C6	-2.73	1.40	1.46
2	A	1104	PTY	O7-C6	-2.72	1.40	1.46
2	B	1103	PTY	O7-C6	-2.71	1.40	1.46
2	A	1110	PTY	O7-C6	-2.70	1.40	1.46
2	C	1101	PTY	O7-C6	-2.69	1.40	1.46
2	C	1106	PTY	O7-C6	-2.67	1.40	1.46
2	A	1107	PTY	O7-C6	-2.67	1.40	1.46
2	C	1104	PTY	O7-C6	-2.67	1.40	1.46
2	C	1109	PTY	O7-C6	-2.66	1.40	1.46
2	A	1111	PTY	O7-C6	-2.64	1.40	1.46
2	C	1110	PTY	O7-C6	-2.63	1.40	1.46
2	B	1109	PTY	O7-C6	-2.62	1.40	1.46
2	B	1105	PTY	O7-C6	-2.61	1.40	1.46
2	B	1108	PTY	O7-C6	-2.61	1.40	1.46
2	B	1106	PTY	O7-C6	-2.60	1.40	1.46
2	A	1103	PTY	O7-C6	-2.58	1.40	1.46
2	B	1102	PTY	O7-C6	-2.56	1.40	1.46
2	B	1101	PTY	O7-C6	-2.55	1.40	1.46
2	B	1104	PTY	O7-C6	-2.52	1.40	1.46
2	A	1105	PTY	O4-C30	2.50	1.40	1.33
2	C	1107	PTY	O4-C30	2.47	1.40	1.33
2	A	1108	PTY	O4-C30	2.46	1.40	1.33
2	B	1102	PTY	O4-C30	2.46	1.40	1.33
2	A	1101	PTY	O7-C8	2.45	1.41	1.34
2	B	1108	PTY	O4-C30	2.45	1.40	1.33
2	C	1108	PTY	O7-C6	-2.44	1.40	1.46
2	B	1105	PTY	O4-C30	2.44	1.40	1.33
2	B	1107	PTY	O4-C30	2.43	1.40	1.33
2	C	1110	PTY	O4-C30	2.43	1.40	1.33
2	B	1104	PTY	O4-C30	2.42	1.40	1.33
2	C	1101	PTY	O4-C30	2.42	1.40	1.33
2	A	1111	PTY	O4-C30	2.41	1.40	1.33
2	B	1109	PTY	O4-C30	2.41	1.40	1.33
2	A	1107	PTY	O4-C30	2.40	1.40	1.33
2	B	1101	PTY	O4-C30	2.39	1.40	1.33
2	A	1103	PTY	O4-C30	2.39	1.40	1.33
2	C	1106	PTY	O4-C30	2.39	1.40	1.33
2	C	1104	PTY	O4-C30	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	PTY	O4-C30	2.38	1.40	1.33
2	C	1108	PTY	O7-C8	2.38	1.41	1.34
2	A	1110	PTY	O4-C30	2.38	1.40	1.33
2	A	1109	PTY	O4-C30	2.37	1.40	1.33
2	C	1103	PTY	O7-C8	2.37	1.40	1.33
2	A	1106	PTY	O4-C30	2.37	1.40	1.33
2	B	1103	PTY	O4-C30	2.37	1.40	1.33
2	A	1107	PTY	O7-C8	2.35	1.40	1.35
2	B	1106	PTY	O4-C30	2.35	1.40	1.33
2	A	1101	PTY	O4-C30	2.34	1.40	1.33
2	A	1101	PTY	O7-C6	-2.34	1.41	1.46
2	C	1109	PTY	O4-C30	2.33	1.40	1.33
2	A	1102	PTY	O7-C8	2.33	1.40	1.34
2	A	1104	PTY	O4-C30	2.30	1.40	1.33
2	A	1102	PTY	O7-C6	-2.29	1.41	1.46
2	B	1104	PTY	O7-C8	2.29	1.40	1.34
2	C	1108	PTY	O4-C30	2.29	1.40	1.33
2	C	1109	PTY	O4-C1	-2.28	1.40	1.45
2	C	1102	PTY	O4-C30	2.28	1.40	1.33
2	B	1105	PTY	O7-C8	2.27	1.40	1.34
2	B	1109	PTY	O7-C8	2.24	1.40	1.34
2	C	1108	PTY	O4-C1	-2.23	1.40	1.45
2	B	1103	PTY	O7-C8	2.23	1.40	1.34
2	A	1103	PTY	O7-C8	2.23	1.40	1.34
2	B	1106	PTY	O4-C1	-2.23	1.40	1.45
2	B	1106	PTY	O7-C8	2.22	1.40	1.34
2	C	1102	PTY	O4-C1	-2.21	1.40	1.45
2	C	1101	PTY	O7-C8	2.21	1.40	1.34
2	A	1111	PTY	O7-C8	2.20	1.40	1.34
2	C	1111	PTY	O4-C30	2.20	1.39	1.33
2	A	1101	PTY	O4-C1	-2.19	1.40	1.45
2	B	1101	PTY	O7-C8	2.19	1.40	1.34
2	B	1102	PTY	O7-C8	2.19	1.40	1.34
2	A	1110	PTY	O7-C8	2.17	1.40	1.34
2	C	1110	PTY	O7-C8	2.17	1.40	1.34
2	A	1104	PTY	O4-C1	-2.16	1.40	1.45
2	C	1109	PTY	O7-C8	2.15	1.40	1.34
2	A	1109	PTY	O4-C1	-2.15	1.40	1.45
2	C	1104	PTY	O7-C8	2.14	1.40	1.34
2	A	1103	PTY	O4-C1	-2.14	1.40	1.45
2	C	1110	PTY	O4-C1	-2.14	1.40	1.45
2	C	1107	PTY	O4-C1	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1103	PTY	O4-C1	-2.13	1.40	1.45
2	C	1102	PTY	O7-C8	2.13	1.40	1.34
2	B	1108	PTY	O7-C8	2.13	1.40	1.34
2	B	1101	PTY	O4-C1	-2.12	1.40	1.45
2	C	1106	PTY	O7-C8	2.11	1.40	1.34
2	C	1101	PTY	O4-C1	-2.10	1.40	1.45
2	B	1107	PTY	O7-C8	2.10	1.40	1.34
2	A	1106	PTY	O7-C8	2.10	1.40	1.34
2	B	1105	PTY	O4-C1	-2.09	1.40	1.45
2	C	1104	PTY	O4-C1	-2.09	1.40	1.45
2	B	1109	PTY	O4-C1	-2.09	1.40	1.45
2	A	1106	PTY	O4-C1	-2.09	1.40	1.45
2	C	1107	PTY	O7-C8	2.08	1.40	1.34
2	C	1106	PTY	O4-C1	-2.08	1.40	1.45
2	A	1111	PTY	O4-C1	-2.07	1.40	1.45
2	A	1109	PTY	O7-C8	2.07	1.40	1.34
2	B	1104	PTY	O4-C1	-2.06	1.40	1.45
2	B	1102	PTY	O4-C1	-2.06	1.40	1.45
2	B	1107	PTY	O4-C1	-2.05	1.40	1.45
2	A	1105	PTY	O7-C8	2.05	1.40	1.34
2	B	1108	PTY	O4-C1	-2.04	1.40	1.45
2	A	1107	PTY	O4-C1	-2.03	1.40	1.45
2	A	1108	PTY	O7-C8	2.03	1.40	1.34
2	A	1108	PTY	O4-C1	-2.02	1.40	1.45
2	A	1102	PTY	O4-C1	-2.02	1.40	1.45
2	A	1105	PTY	O4-C1	-2.02	1.40	1.45
2	A	1104	PTY	O7-C8	2.02	1.40	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1107	PTY	O7-C8-C11	5.16	120.28	111.09
2	A	1102	PTY	O7-C8-C11	4.75	121.76	111.48
2	C	1108	PTY	O7-C8-C11	4.73	121.72	111.48
2	A	1101	PTY	O7-C8-C11	4.70	121.64	111.48
2	B	1109	PTY	O7-C8-C11	4.33	120.86	111.48
2	B	1102	PTY	O7-C8-C11	4.28	120.74	111.48
2	C	1109	PTY	O7-C8-C11	4.23	120.64	111.48
2	A	1103	PTY	O7-C8-C11	4.19	120.54	111.48
2	B	1104	PTY	O7-C8-C11	4.16	120.48	111.48
2	C	1102	PTY	O7-C8-C11	4.13	120.41	111.48
2	C	1110	PTY	O7-C8-C11	4.11	120.38	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1106	PTY	O7-C8-C11	4.11	120.37	111.48
2	C	1106	PTY	O7-C8-C11	4.07	120.28	111.48
2	B	1101	PTY	O7-C8-C11	4.06	120.25	111.48
2	C	1104	PTY	O7-C8-C11	4.00	120.12	111.48
2	C	1107	PTY	O7-C8-C11	3.99	120.11	111.48
2	A	1111	PTY	O7-C8-C11	3.99	120.10	111.48
2	A	1109	PTY	O7-C8-C11	3.92	119.97	111.48
2	C	1101	PTY	O7-C8-C11	3.91	119.94	111.48
2	A	1110	PTY	O7-C8-C11	3.88	119.87	111.48
2	A	1105	PTY	O7-C8-C11	3.86	119.83	111.48
2	B	1107	PTY	O7-C8-C11	3.86	119.83	111.48
2	A	1106	PTY	O7-C8-C11	3.86	119.83	111.48
2	A	1104	PTY	O7-C8-C11	3.84	119.79	111.48
2	B	1108	PTY	O7-C8-C11	3.81	119.73	111.48
2	A	1108	PTY	O7-C8-C11	3.57	119.21	111.48
2	B	1103	PTY	O7-C8-C11	3.47	118.98	111.48
2	B	1105	PTY	O7-C8-C11	3.33	118.68	111.48
2	B	1107	PTY	O4-C30-C31	3.15	121.45	111.83
2	C	1103	PTY	O7-C8-C11	2.96	120.87	111.83
2	B	1102	PTY	O4-C30-C31	2.92	120.74	111.83
2	A	1107	PTY	O4-C30-C31	2.92	120.73	111.83
2	B	1103	PTY	O4-C30-C31	2.86	120.56	111.83
2	B	1101	PTY	O4-C30-C31	2.84	120.50	111.83
2	C	1102	PTY	O4-C30-C31	2.82	120.44	111.83
2	A	1102	PTY	O4-C30-C31	2.78	120.30	111.83
2	C	1107	PTY	O4-C30-C31	2.76	120.26	111.83
2	A	1108	PTY	O4-C30-C31	2.74	120.20	111.83
2	A	1103	PTY	O4-C30-C31	2.73	120.17	111.83
2	A	1110	PTY	O4-C30-C31	2.73	119.43	111.15
2	B	1104	PTY	O4-C30-C31	2.73	120.15	111.83
2	A	1106	PTY	O4-C30-C31	2.71	120.09	111.83
2	C	1106	PTY	O4-C30-C31	2.71	120.09	111.83
2	B	1108	PTY	O4-C30-C31	2.70	120.08	111.83
2	A	1109	PTY	O4-C30-C31	2.70	120.07	111.83
2	A	1104	PTY	O4-C30-C31	2.70	120.06	111.83
2	A	1101	PTY	O4-C30-C31	2.67	119.96	111.83
2	C	1104	PTY	O4-C30-C31	2.64	119.89	111.83
2	C	1101	PTY	O4-C30-C31	2.64	119.88	111.83
2	C	1111	PTY	O4-C30-C31	2.60	119.77	111.83
2	C	1109	PTY	O4-C30-C31	2.54	119.59	111.83
2	C	1108	PTY	O4-C30-C31	2.54	119.59	111.83
2	A	1111	PTY	O4-C30-C31	2.49	119.43	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1105	PTY	O4-C30-C31	2.49	119.42	111.83
2	B	1109	PTY	O4-C30-C31	2.45	119.30	111.83
2	B	1106	PTY	O4-C30-C31	2.44	119.26	111.83
2	C	1110	PTY	O4-C30-C31	2.40	119.15	111.83
2	A	1105	PTY	O4-C30-C31	2.38	119.08	111.83
2	A	1108	PTY	C6-O7-C8	-2.10	112.77	117.80
2	A	1109	PTY	C6-O7-C8	-2.05	112.88	117.80

There are no chirality outliers.

All (510) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	PTY	C5-O14-P1-O11
2	B	1101	PTY	C5-O14-P1-O12
2	B	1103	PTY	C3-O11-P1-O12
2	B	1103	PTY	C3-O11-P1-O14
2	B	1103	PTY	C5-O14-P1-O11
2	B	1103	PTY	C5-O14-P1-O12
2	B	1103	PTY	C5-O14-P1-O13
2	B	1104	PTY	O4-C1-C6-O7
2	B	1104	PTY	C5-O14-P1-O11
2	B	1104	PTY	C5-O14-P1-O13
2	B	1105	PTY	O4-C1-C6-O7
2	B	1105	PTY	O14-C5-C6-C1
2	B	1105	PTY	O14-C5-C6-O7
2	B	1106	PTY	N1-C2-C3-O11
2	B	1106	PTY	C5-O14-P1-O11
2	B	1106	PTY	C5-O14-P1-O12
2	B	1106	PTY	C5-O14-P1-O13
2	B	1107	PTY	C3-O11-P1-O13
2	B	1107	PTY	C3-O11-P1-O14
2	B	1108	PTY	N1-C2-C3-O11
2	B	1108	PTY	C5-O14-P1-O11
2	B	1108	PTY	C5-O14-P1-O13
2	B	1109	PTY	N1-C2-C3-O11
2	B	1109	PTY	O10-C8-O7-C6
2	B	1109	PTY	C11-C8-O7-C6
2	B	1109	PTY	C3-O11-P1-O12
2	B	1109	PTY	C3-O11-P1-O13
2	B	1109	PTY	C3-O11-P1-O14
2	B	1109	PTY	C5-O14-P1-O11
2	B	1109	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
2	B	1109	PTY	C5-O14-P1-O13
2	C	1101	PTY	C3-O11-P1-O13
2	C	1101	PTY	C5-O14-P1-O11
2	C	1101	PTY	C5-O14-P1-O12
2	C	1101	PTY	C5-O14-P1-O13
2	C	1102	PTY	N1-C2-C3-O11
2	C	1102	PTY	C5-O14-P1-O11
2	C	1102	PTY	C5-O14-P1-O12
2	C	1103	PTY	N1-C2-C3-O11
2	C	1103	PTY	O14-C5-C6-O7
2	C	1103	PTY	C3-O11-P1-O13
2	C	1103	PTY	C3-O11-P1-O14
2	C	1104	PTY	C3-O11-P1-O12
2	C	1104	PTY	C3-O11-P1-O13
2	C	1104	PTY	C3-O11-P1-O14
2	C	1106	PTY	O4-C1-C6-O7
2	C	1106	PTY	N1-C2-C3-O11
2	C	1106	PTY	C5-O14-P1-O11
2	C	1106	PTY	C5-O14-P1-O12
2	C	1107	PTY	N1-C2-C3-O11
2	C	1107	PTY	C3-O11-P1-O13
2	C	1107	PTY	C3-O11-P1-O14
2	C	1108	PTY	O10-C8-O7-C6
2	C	1108	PTY	C11-C8-O7-C6
2	C	1108	PTY	C3-O11-P1-O14
2	C	1108	PTY	C5-O14-P1-O11
2	C	1108	PTY	C5-O14-P1-O13
2	C	1109	PTY	O4-C1-C6-O7
2	C	1109	PTY	C3-O11-P1-O12
2	C	1109	PTY	C3-O11-P1-O13
2	C	1109	PTY	C3-O11-P1-O14
2	C	1109	PTY	C5-O14-P1-O11
2	C	1109	PTY	C5-O14-P1-O12
2	C	1110	PTY	O14-C5-C6-O7
2	C	1110	PTY	O10-C8-O7-C6
2	C	1110	PTY	C11-C8-O7-C6
2	C	1111	PTY	C3-O11-P1-O12
2	C	1111	PTY	C3-O11-P1-O13
2	C	1111	PTY	C3-O11-P1-O14
2	A	1101	PTY	C11-C8-O7-C6
2	A	1101	PTY	C3-O11-P1-O13
2	A	1101	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
2	A	1102	PTY	O10-C8-O7-C6
2	A	1102	PTY	C11-C8-O7-C6
2	A	1104	PTY	C3-O11-P1-O12
2	A	1104	PTY	C3-O11-P1-O13
2	A	1104	PTY	C3-O11-P1-O14
2	A	1104	PTY	C5-O14-P1-O11
2	A	1104	PTY	C5-O14-P1-O12
2	A	1104	PTY	C5-O14-P1-O13
2	A	1105	PTY	C3-O11-P1-O13
2	A	1105	PTY	C3-O11-P1-O14
2	A	1106	PTY	O4-C1-C6-O7
2	A	1106	PTY	N1-C2-C3-O11
2	A	1106	PTY	O10-C8-O7-C6
2	A	1106	PTY	C5-O14-P1-O11
2	A	1106	PTY	C5-O14-P1-O12
2	A	1107	PTY	C5-O14-P1-O11
2	A	1107	PTY	C5-O14-P1-O12
2	A	1107	PTY	C5-O14-P1-O13
2	A	1108	PTY	O10-C8-O7-C6
2	A	1108	PTY	C11-C8-O7-C6
2	A	1108	PTY	C5-O14-P1-O11
2	A	1108	PTY	C5-O14-P1-O12
2	A	1108	PTY	C5-O14-P1-O13
2	A	1109	PTY	C3-O11-P1-O14
2	A	1109	PTY	C5-O14-P1-O11
2	A	1109	PTY	C5-O14-P1-O12
2	A	1110	PTY	C5-O14-P1-O11
2	A	1110	PTY	C5-O14-P1-O12
2	A	1110	PTY	C5-O14-P1-O13
2	A	1111	PTY	N1-C2-C3-O11
2	A	1111	PTY	C3-O11-P1-O12
2	A	1111	PTY	C3-O11-P1-O13
2	A	1111	PTY	C5-O14-P1-O13
2	A	1107	PTY	C11-C8-O7-C6
2	C	1103	PTY	O10-C8-O7-C6
2	C	1103	PTY	C11-C8-O7-C6
2	B	1101	PTY	O30-C30-O4-C1
2	B	1103	PTY	O30-C30-O4-C1
2	B	1106	PTY	O30-C30-O4-C1
2	C	1104	PTY	O30-C30-O4-C1
2	C	1107	PTY	O30-C30-O4-C1
2	A	1102	PTY	O30-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
2	A	1104	PTY	O30-C30-O4-C1
2	A	1106	PTY	O30-C30-O4-C1
2	A	1110	PTY	O30-C30-O4-C1
2	B	1104	PTY	O10-C8-O7-C6
2	B	1108	PTY	O10-C8-O7-C6
2	A	1101	PTY	O10-C8-O7-C6
2	B	1101	PTY	C31-C30-O4-C1
2	B	1103	PTY	C31-C30-O4-C1
2	B	1107	PTY	C31-C30-O4-C1
2	C	1104	PTY	C31-C30-O4-C1
2	A	1102	PTY	C31-C30-O4-C1
2	A	1104	PTY	C31-C30-O4-C1
2	A	1106	PTY	C31-C30-O4-C1
2	A	1108	PTY	C31-C30-O4-C1
2	A	1110	PTY	C31-C30-O4-C1
2	B	1104	PTY	C11-C8-O7-C6
2	B	1108	PTY	C11-C8-O7-C6
2	A	1106	PTY	C11-C8-O7-C6
2	A	1107	PTY	O10-C8-O7-C6
2	B	1106	PTY	C31-C30-O4-C1
2	C	1107	PTY	C31-C30-O4-C1
2	B	1107	PTY	O30-C30-O4-C1
2	A	1108	PTY	O30-C30-O4-C1
2	B	1107	PTY	C11-C8-O7-C6
2	A	1111	PTY	C11-C8-O7-C6
2	C	1108	PTY	C31-C30-O4-C1
2	C	1108	PTY	O30-C30-O4-C1
2	A	1111	PTY	O10-C8-O7-C6
2	C	1107	PTY	O14-C5-C6-O7
2	C	1102	PTY	C11-C8-O7-C6
2	B	1107	PTY	O10-C8-O7-C6
2	B	1105	PTY	C8-C11-C12-C13
2	C	1101	PTY	C30-C31-C32-C33
2	A	1105	PTY	C11-C8-O7-C6
2	A	1109	PTY	C11-C8-O7-C6
2	B	1107	PTY	C8-C11-C12-C13
2	A	1107	PTY	C31-C30-O4-C1
2	B	1106	PTY	C11-C8-O7-C6
2	C	1104	PTY	C11-C8-O7-C6
2	B	1106	PTY	O10-C8-O7-C6
2	C	1102	PTY	O10-C8-O7-C6
2	A	1104	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
2	A	1105	PTY	O10-C8-O7-C6
2	A	1109	PTY	O10-C8-O7-C6
2	C	1107	PTY	C11-C8-O7-C6
2	A	1104	PTY	C11-C8-O7-C6
2	A	1110	PTY	C11-C8-O7-C6
2	C	1104	PTY	O10-C8-O7-C6
2	A	1110	PTY	O10-C8-O7-C6
2	C	1111	PTY	O14-C5-C6-C1
2	A	1107	PTY	O30-C30-O4-C1
2	B	1102	PTY	C11-C8-O7-C6
2	A	1106	PTY	C30-C31-C32-C33
2	C	1101	PTY	C33-C34-C35-C36
2	C	1103	PTY	C15-C16-C17-C18
2	C	1110	PTY	C15-C16-C17-C18
2	C	1111	PTY	C30-C31-C32-C33
2	C	1106	PTY	C34-C35-C36-C37
2	B	1105	PTY	C11-C12-C13-C14
2	B	1106	PTY	C15-C16-C17-C18
2	B	1108	PTY	C11-C12-C13-C14
2	B	1108	PTY	C32-C33-C34-C35
2	C	1104	PTY	C13-C14-C15-C16
2	C	1106	PTY	C35-C36-C37-C38
2	C	1108	PTY	C11-C12-C13-C14
2	C	1110	PTY	C32-C33-C34-C35
2	A	1101	PTY	C25-C26-C27-C28
2	C	1107	PTY	O10-C8-O7-C6
2	C	1101	PTY	C32-C33-C34-C35
2	A	1102	PTY	C13-C14-C15-C16
2	A	1103	PTY	C16-C17-C18-C19
2	A	1103	PTY	C31-C32-C33-C34
2	C	1102	PTY	C8-C11-C12-C13
2	C	1108	PTY	C33-C34-C35-C36
2	B	1106	PTY	C14-C15-C16-C17
2	B	1104	PTY	C15-C16-C17-C18
3	C	1115	D12	C6-C7-C8-C9
2	B	1108	PTY	C8-C11-C12-C13
2	B	1107	PTY	C31-C32-C33-C34
3	C	1116	D12	C5-C6-C7-C8
2	A	1110	PTY	C14-C15-C16-C17
2	C	1104	PTY	C14-C15-C16-C17
2	A	1107	PTY	O4-C1-C6-C5
2	B	1105	PTY	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	1107	PTY	C31-C32-C33-C34
2	B	1109	PTY	C8-C11-C12-C13
2	C	1104	PTY	C11-C12-C13-C14
2	C	1106	PTY	C33-C34-C35-C36
2	A	1103	PTY	C33-C34-C35-C36
2	B	1101	PTY	C40-C41-C42-C43
2	B	1104	PTY	C11-C12-C13-C14
2	B	1107	PTY	C15-C16-C17-C18
2	A	1101	PTY	C34-C35-C36-C37
2	A	1104	PTY	C11-C12-C13-C14
2	C	1109	PTY	C30-C31-C32-C33
2	A	1106	PTY	C32-C33-C34-C35
2	B	1102	PTY	O10-C8-O7-C6
3	B	1110	D12	C4-C5-C6-C7
2	A	1107	PTY	C35-C36-C37-C38
2	B	1102	PTY	C30-C31-C32-C33
2	C	1106	PTY	C31-C30-O4-C1
2	B	1101	PTY	C39-C40-C41-C42
2	C	1108	PTY	C31-C32-C33-C34
2	A	1102	PTY	C16-C17-C18-C19
3	C	1115	D12	C3-C4-C5-C6
2	A	1108	PTY	C13-C14-C15-C16
2	A	1104	PTY	C17-C18-C19-C20
2	C	1109	PTY	C11-C8-O7-C6
2	A	1111	PTY	C30-C31-C32-C33
2	A	1101	PTY	C12-C13-C14-C15
2	B	1101	PTY	C8-C11-C12-C13
2	A	1101	PTY	C39-C40-C41-C42
2	B	1106	PTY	C22-C23-C24-C25
2	B	1101	PTY	C11-C12-C13-C14
2	A	1101	PTY	C14-C15-C16-C17
2	B	1102	PTY	C11-C12-C13-C14
2	A	1111	PTY	C37-C38-C39-C40
2	A	1111	PTY	O14-C5-C6-O7
3	C	1113	D12	C4-C5-C6-C7
2	B	1103	PTY	C13-C14-C15-C16
2	C	1103	PTY	C8-C11-C12-C13
2	A	1109	PTY	C30-C31-C32-C33
2	A	1111	PTY	C15-C16-C17-C18
2	B	1101	PTY	C36-C37-C38-C39
2	A	1101	PTY	C37-C38-C39-C40
2	A	1103	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
3	B	1110	D12	C6-C7-C8-C9
2	B	1106	PTY	C32-C33-C34-C35
2	B	1107	PTY	C11-C12-C13-C14
2	A	1104	PTY	C32-C33-C34-C35
2	C	1102	PTY	C32-C33-C34-C35
2	A	1107	PTY	C40-C41-C42-C43
2	C	1105	PTY	C12-C13-C14-C15
2	B	1106	PTY	C18-C19-C20-C21
2	A	1103	PTY	C34-C35-C36-C37
2	C	1104	PTY	O14-C5-C6-C1
2	C	1107	PTY	O14-C5-C6-C1
2	C	1110	PTY	O14-C5-C6-C1
2	C	1109	PTY	O10-C8-O7-C6
2	C	1108	PTY	C30-C31-C32-C33
2	B	1106	PTY	C23-C24-C25-C26
2	C	1106	PTY	O30-C30-O4-C1
3	B	1113	D12	C6-C7-C8-C9
2	B	1102	PTY	O4-C1-C6-C5
2	C	1106	PTY	O4-C1-C6-C5
2	A	1103	PTY	O4-C1-C6-C5
2	A	1106	PTY	O4-C1-C6-C5
2	A	1108	PTY	O4-C1-C6-C5
2	C	1110	PTY	C36-C37-C38-C39
2	C	1102	PTY	C17-C18-C19-C20
2	C	1106	PTY	C17-C18-C19-C20
2	C	1107	PTY	C17-C18-C19-C20
2	A	1103	PTY	O30-C30-O4-C1
2	C	1106	PTY	C14-C15-C16-C17
3	B	1115	D12	C7-C8-C9-C10
2	A	1106	PTY	C31-C32-C33-C34
2	A	1109	PTY	C12-C13-C14-C15
2	A	1101	PTY	C35-C36-C37-C38
2	B	1108	PTY	O14-C5-C6-O7
2	C	1102	PTY	O14-C5-C6-O7
2	C	1106	PTY	C37-C38-C39-C40
2	B	1109	PTY	C34-C35-C36-C37
2	C	1101	PTY	C35-C36-C37-C38
2	A	1105	PTY	C12-C13-C14-C15
2	A	1111	PTY	C19-C20-C21-C22
2	A	1102	PTY	C11-C12-C13-C14
2	A	1107	PTY	C41-C42-C43-C44
2	A	1108	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	C21-C22-C23-C24
2	A	1104	PTY	C6-C5-O14-P1
2	A	1108	PTY	C6-C5-O14-P1
2	A	1109	PTY	C36-C37-C38-C39
2	B	1109	PTY	C39-C40-C41-C42
2	B	1104	PTY	C14-C15-C16-C17
2	A	1103	PTY	C17-C18-C19-C20
2	C	1102	PTY	O14-C5-C6-C1
2	A	1101	PTY	O14-C5-C6-C1
2	A	1111	PTY	O14-C5-C6-C1
2	C	1105	PTY	C11-C12-C13-C14
2	C	1111	PTY	C31-C30-O4-C1
2	A	1101	PTY	C36-C37-C38-C39
3	B	1110	D12	C11-C10-C9-C8
2	C	1108	PTY	C14-C15-C16-C17
2	B	1101	PTY	O4-C1-C6-C5
2	B	1103	PTY	O4-C1-C6-C5
2	B	1104	PTY	O4-C1-C6-C5
2	C	1109	PTY	O4-C1-C6-C5
2	B	1109	PTY	C36-C37-C38-C39
2	A	1104	PTY	C31-C32-C33-C34
2	B	1101	PTY	O14-C5-C6-O7
2	C	1101	PTY	O14-C5-C6-O7
2	A	1101	PTY	O14-C5-C6-O7
2	A	1108	PTY	O14-C5-C6-O7
2	A	1109	PTY	O14-C5-C6-O7
2	A	1110	PTY	C12-C13-C14-C15
2	C	1107	PTY	C6-C5-O14-P1
2	B	1103	PTY	C11-C12-C13-C14
2	B	1101	PTY	O4-C1-C6-O7
3	B	1113	D12	C1-C2-C3-C4
2	C	1110	PTY	C34-C35-C36-C37
2	B	1105	PTY	C12-C11-C8-O7
2	C	1101	PTY	C31-C32-C33-C34
2	B	1108	PTY	O14-C5-C6-C1
2	A	1110	PTY	O14-C5-C6-C1
2	A	1110	PTY	C17-C18-C19-C20
2	C	1103	PTY	C16-C17-C18-C19
2	A	1103	PTY	C11-C12-C13-C14
3	C	1115	D12	C4-C5-C6-C7
2	B	1103	PTY	C8-C11-C12-C13
3	B	1110	D12	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	1104	PTY	C30-C31-C32-C33
2	C	1111	PTY	C35-C36-C37-C38
2	C	1109	PTY	O14-C5-C6-O7
2	C	1111	PTY	C37-C38-C39-C40
2	C	1111	PTY	O30-C30-O4-C1
2	A	1101	PTY	C33-C34-C35-C36
2	B	1109	PTY	C38-C39-C40-C41
2	C	1111	PTY	C33-C34-C35-C36
2	B	1103	PTY	O4-C1-C6-O7
2	A	1103	PTY	O4-C1-C6-O7
2	A	1107	PTY	O4-C1-C6-O7
2	A	1106	PTY	C12-C13-C14-C15
2	B	1108	PTY	C35-C36-C37-C38
3	C	1116	D12	C6-C7-C8-C9
2	C	1108	PTY	C8-C11-C12-C13
2	A	1106	PTY	C39-C40-C41-C42
2	A	1101	PTY	C18-C19-C20-C21
2	B	1109	PTY	C11-C12-C13-C14
2	C	1109	PTY	C15-C16-C17-C18
2	A	1111	PTY	C36-C37-C38-C39
2	B	1101	PTY	C37-C38-C39-C40
2	C	1102	PTY	C35-C36-C37-C38
2	C	1107	PTY	C15-C16-C17-C18
2	A	1110	PTY	C13-C14-C15-C16
2	B	1101	PTY	O14-C5-C6-C1
2	C	1101	PTY	O14-C5-C6-C1
2	C	1108	PTY	O14-C5-C6-C1
2	A	1109	PTY	C13-C14-C15-C16
2	B	1109	PTY	C14-C15-C16-C17
2	C	1111	PTY	C32-C33-C34-C35
2	B	1109	PTY	C32-C33-C34-C35
2	C	1108	PTY	O14-C5-C6-O7
2	A	1110	PTY	O14-C5-C6-O7
2	B	1107	PTY	C35-C36-C37-C38
2	B	1102	PTY	O4-C1-C6-O7
2	C	1104	PTY	O4-C1-C6-O7
2	A	1108	PTY	O4-C1-C6-O7
2	B	1105	PTY	O4-C1-C6-C5
2	B	1109	PTY	O4-C1-C6-C5
2	B	1101	PTY	C30-C31-C32-C33
2	A	1105	PTY	C16-C17-C18-C19
2	A	1107	PTY	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	B	1101	PTY	C5-O14-P1-O13
2	B	1102	PTY	C5-O14-P1-O11
2	B	1102	PTY	C5-O14-P1-O13
2	B	1103	PTY	C3-O11-P1-O13
2	B	1104	PTY	N1-C2-C3-O11
2	B	1104	PTY	C5-O14-P1-O12
2	B	1107	PTY	C3-O11-P1-O12
2	B	1107	PTY	C5-O14-P1-O11
2	B	1107	PTY	C5-O14-P1-O12
2	B	1108	PTY	C5-O14-P1-O12
2	C	1104	PTY	C5-O14-P1-O11
2	C	1104	PTY	C5-O14-P1-O12
2	C	1104	PTY	C5-O14-P1-O13
2	C	1106	PTY	C5-O14-P1-O13
2	C	1107	PTY	C3-O11-P1-O12
2	C	1109	PTY	C5-O14-P1-O13
2	C	1110	PTY	N1-C2-C3-O11
2	C	1110	PTY	C5-O14-P1-O11
2	A	1101	PTY	N1-C2-C3-O11
2	A	1101	PTY	C5-O14-P1-O11
2	A	1102	PTY	C5-O14-P1-O11
2	A	1102	PTY	C5-O14-P1-O12
2	A	1102	PTY	C5-O14-P1-O13
2	A	1103	PTY	N1-C2-C3-O11
2	A	1103	PTY	C3-O11-P1-O13
2	A	1103	PTY	C5-O14-P1-O12
2	A	1107	PTY	C3-O11-P1-O12
2	A	1109	PTY	C3-O11-P1-O13
2	A	1110	PTY	C3-O11-P1-O13
2	A	1111	PTY	C3-O11-P1-O14
2	A	1111	PTY	C5-O14-P1-O11
2	A	1111	PTY	C5-O14-P1-O12
2	A	1101	PTY	C38-C39-C40-C41
2	A	1111	PTY	C11-C12-C13-C14
2	B	1104	PTY	C6-C5-O14-P1
2	B	1107	PTY	C6-C5-O14-P1
2	B	1109	PTY	C6-C5-O14-P1
2	C	1101	PTY	C6-C5-O14-P1
2	A	1101	PTY	C12-C11-C8-O7
2	B	1101	PTY	C34-C35-C36-C37
2	C	1110	PTY	C12-C13-C14-C15
2	B	1108	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	A	1102	PTY	C1-C6-O7-C8
2	B	1109	PTY	O14-C5-C6-C1
2	C	1104	PTY	O14-C5-C6-O7
2	A	1105	PTY	O14-C5-C6-O7
3	B	1114	D12	C3-C4-C5-C6
3	B	1114	D12	C2-C3-C4-C5
2	C	1111	PTY	C31-C32-C33-C34
2	B	1108	PTY	O4-C1-C6-O7
2	C	1108	PTY	O4-C1-C6-O7
2	C	1101	PTY	C34-C35-C36-C37
3	B	1112	D12	C3-C4-C5-C6
2	A	1104	PTY	C40-C41-C42-C43
3	C	1115	D12	C5-C6-C7-C8
2	C	1106	PTY	C11-C8-O7-C6
2	B	1108	PTY	C15-C16-C17-C18
2	A	1111	PTY	C35-C36-C37-C38
2	A	1101	PTY	C31-C32-C33-C34
2	A	1109	PTY	C38-C39-C40-C41
2	A	1109	PTY	C33-C34-C35-C36
2	C	1106	PTY	O10-C8-O7-C6
2	C	1106	PTY	C32-C33-C34-C35
2	B	1106	PTY	C6-C5-O14-P1
2	A	1109	PTY	C6-C5-O14-P1
2	B	1108	PTY	C33-C34-C35-C36
2	C	1110	PTY	O4-C1-C6-C5
2	C	1105	PTY	C18-C19-C20-C21
2	C	1104	PTY	C8-C11-C12-C13
2	A	1104	PTY	C1-C6-O7-C8
2	A	1104	PTY	C5-C6-O7-C8
2	C	1105	PTY	C13-C14-C15-C16
2	A	1110	PTY	C15-C16-C17-C18
2	C	1107	PTY	C13-C14-C15-C16
2	C	1102	PTY	C6-C5-O14-P1
2	C	1109	PTY	C6-C5-O14-P1
2	C	1109	PTY	O14-C5-C6-C1
2	A	1105	PTY	O14-C5-C6-C1
2	A	1108	PTY	O14-C5-C6-C1
2	C	1111	PTY	C34-C35-C36-C37
2	A	1105	PTY	O4-C1-C6-O7
2	C	1110	PTY	C13-C14-C15-C16
2	A	1104	PTY	C19-C20-C21-C22
2	A	1109	PTY	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	C31-C30-O4-C1
2	C	1105	PTY	C15-C16-C17-C18
2	B	1105	PTY	C39-C40-C41-C42
2	B	1101	PTY	C35-C36-C37-C38
2	C	1108	PTY	O4-C1-C6-C5
3	B	1112	D12	C4-C5-C6-C7
2	B	1109	PTY	O14-C5-C6-O7
2	C	1110	PTY	C31-C32-C33-C34
2	A	1101	PTY	O30-C30-O4-C1
2	A	1109	PTY	O14-C5-C6-C1
2	C	1111	PTY	C36-C37-C38-C39
2	C	1108	PTY	C12-C13-C14-C15
2	B	1104	PTY	C13-C14-C15-C16
2	B	1106	PTY	C11-C12-C13-C14
3	B	1114	D12	C4-C5-C6-C7
2	A	1109	PTY	C8-C11-C12-C13
2	B	1107	PTY	C36-C37-C38-C39
2	C	1109	PTY	C12-C11-C8-O7
2	B	1102	PTY	C12-C11-C8-O7
2	C	1103	PTY	C11-C12-C13-C14
2	B	1101	PTY	C6-C5-O14-P1
2	C	1104	PTY	O4-C1-C6-C5
2	A	1109	PTY	C11-C12-C13-C14
2	B	1109	PTY	C35-C36-C37-C38
2	B	1103	PTY	C31-C32-C33-C34
2	A	1105	PTY	C12-C11-C8-O7
2	A	1109	PTY	C37-C38-C39-C40
2	C	1104	PTY	C32-C33-C34-C35
2	B	1109	PTY	C16-C17-C18-C19
2	A	1105	PTY	C8-C11-C12-C13
2	A	1111	PTY	C31-C32-C33-C34
2	B	1105	PTY	C12-C11-C8-O10
2	B	1108	PTY	O4-C30-C31-C32
2	C	1108	PTY	C12-C11-C8-O7
2	C	1101	PTY	C13-C14-C15-C16
2	A	1106	PTY	C12-C11-C8-O7
2	B	1108	PTY	O4-C1-C6-C5
2	A	1106	PTY	O4-C30-C31-C32
2	A	1111	PTY	O4-C1-C6-O7
2	B	1108	PTY	C12-C11-C8-O7
3	B	1113	D12	C2-C3-C4-C5
2	A	1107	PTY	C1-C6-O7-C8

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Mol	Chain	Res	Type	Atoms
2	A	1107	PTY	C5-C6-O7-C8
2	C	1104	PTY	C6-C5-O14-P1
2	A	1102	PTY	O4-C30-C31-C32
2	C	1106	PTY	C13-C14-C15-C16
2	A	1110	PTY	C8-C11-C12-C13
2	B	1108	PTY	O30-C30-C31-C32
2	A	1105	PTY	C12-C11-C8-O10
2	A	1106	PTY	C12-C11-C8-O10
2	C	1108	PTY	C12-C11-C8-O10
2	B	1106	PTY	O4-C1-C6-C5
2	A	1110	PTY	O4-C1-C6-C5
2	C	1111	PTY	O4-C30-C31-C32
2	B	1108	PTY	C12-C11-C8-O10
2	A	1102	PTY	O30-C30-C31-C32
3	B	1115	D12	C1-C2-C3-C4
2	B	1107	PTY	C34-C35-C36-C37
2	A	1106	PTY	O30-C30-C31-C32
2	A	1110	PTY	C12-C11-C8-O7

There are no ring outliers.

25 monomers are involved in 36 short contacts:

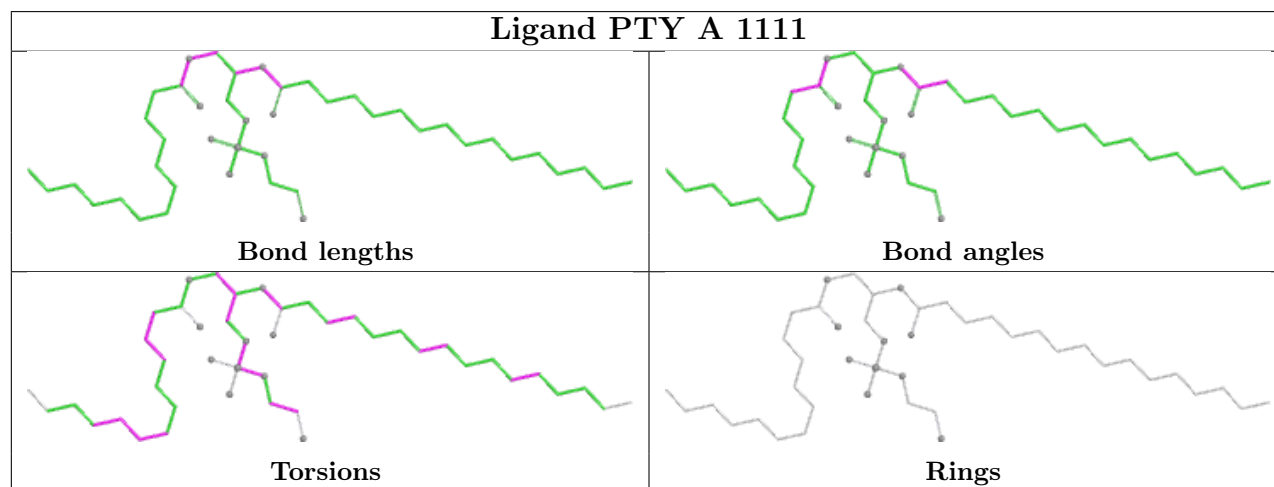
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1111	PTY	3	0
2	B	1105	PTY	1	0
2	B	1106	PTY	3	0
3	C	1113	D12	2	0
3	C	1114	D12	1	0
2	C	1102	PTY	3	0
2	A	1104	PTY	1	0
2	B	1108	PTY	1	0
2	A	1108	PTY	2	0
2	C	1103	PTY	1	0
2	B	1107	PTY	2	0
3	C	1116	D12	3	0
2	C	1110	PTY	4	0
2	C	1111	PTY	1	0
2	C	1101	PTY	4	0
2	A	1101	PTY	2	0
2	C	1104	PTY	1	0
3	B	1110	D12	1	0
2	B	1101	PTY	1	0

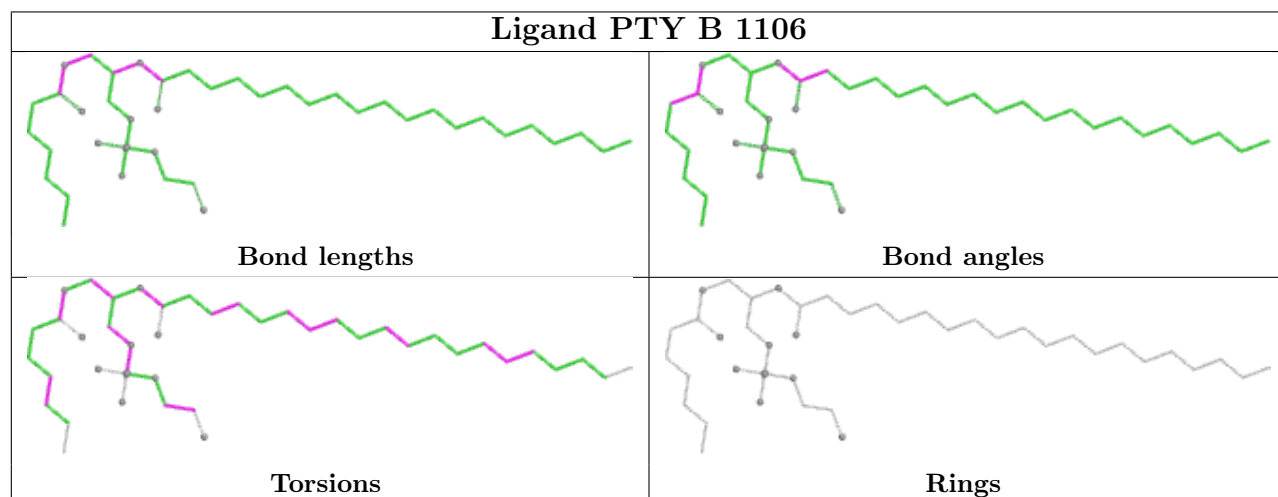
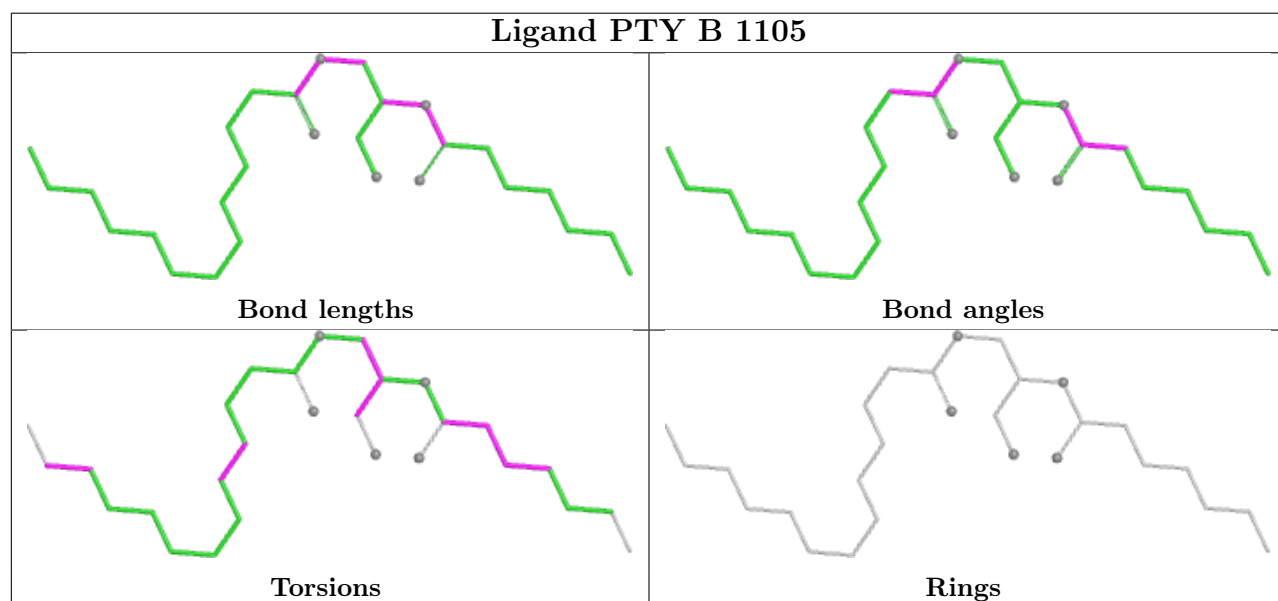
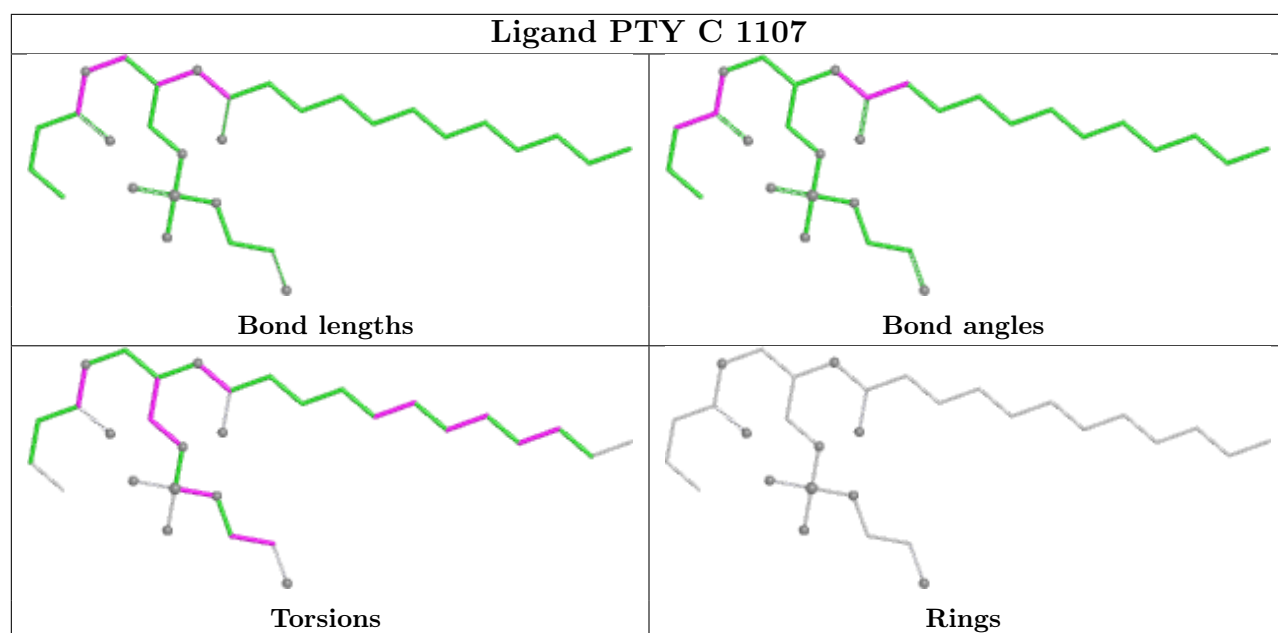
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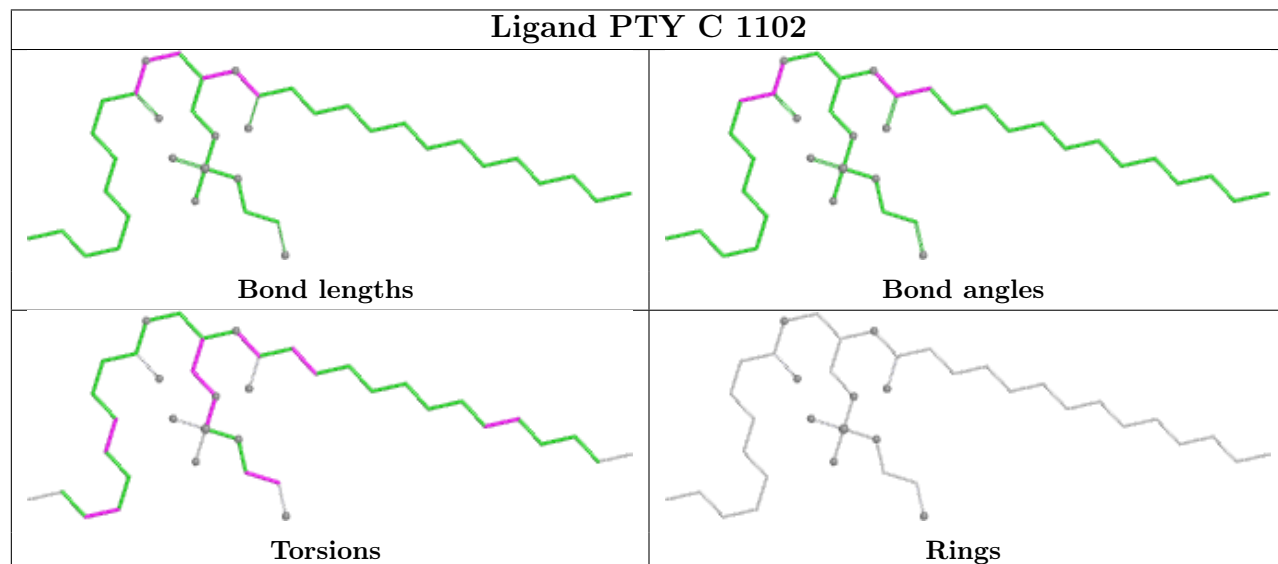
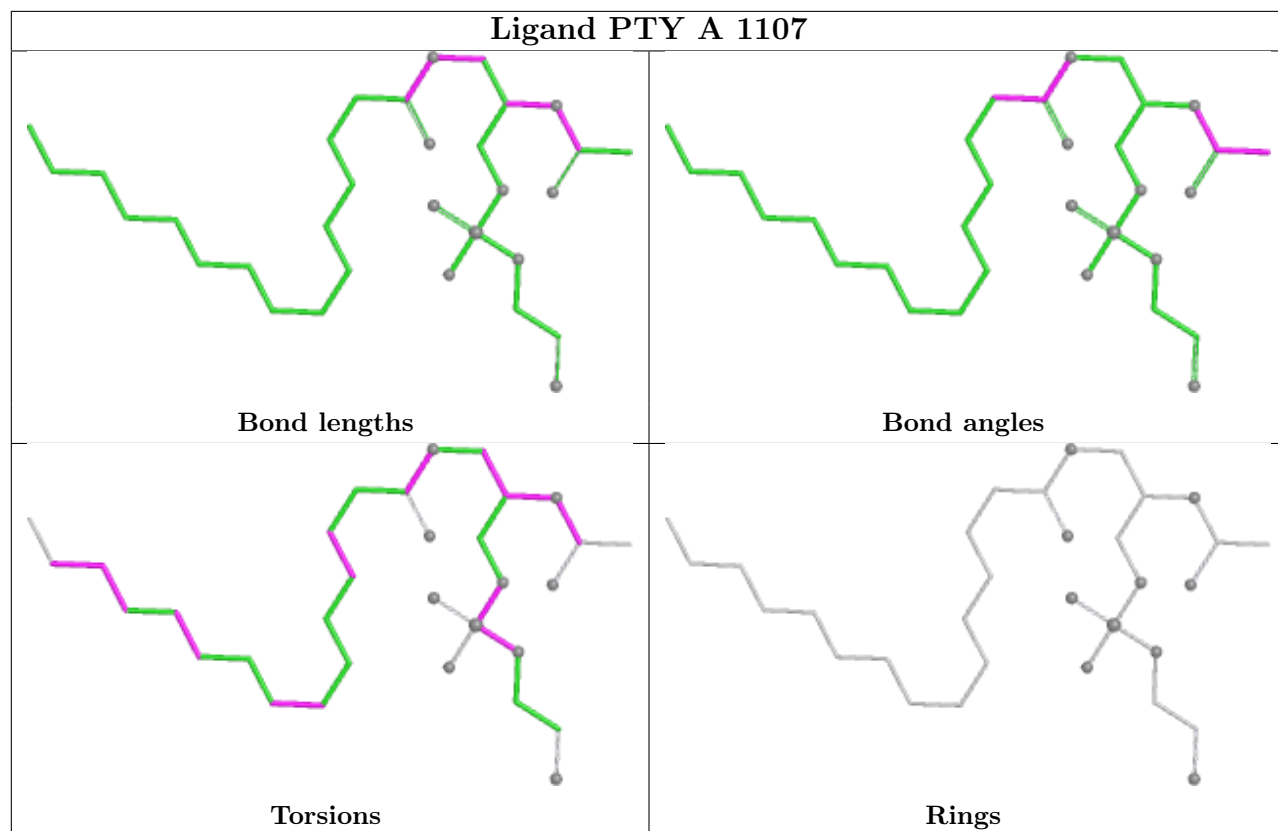
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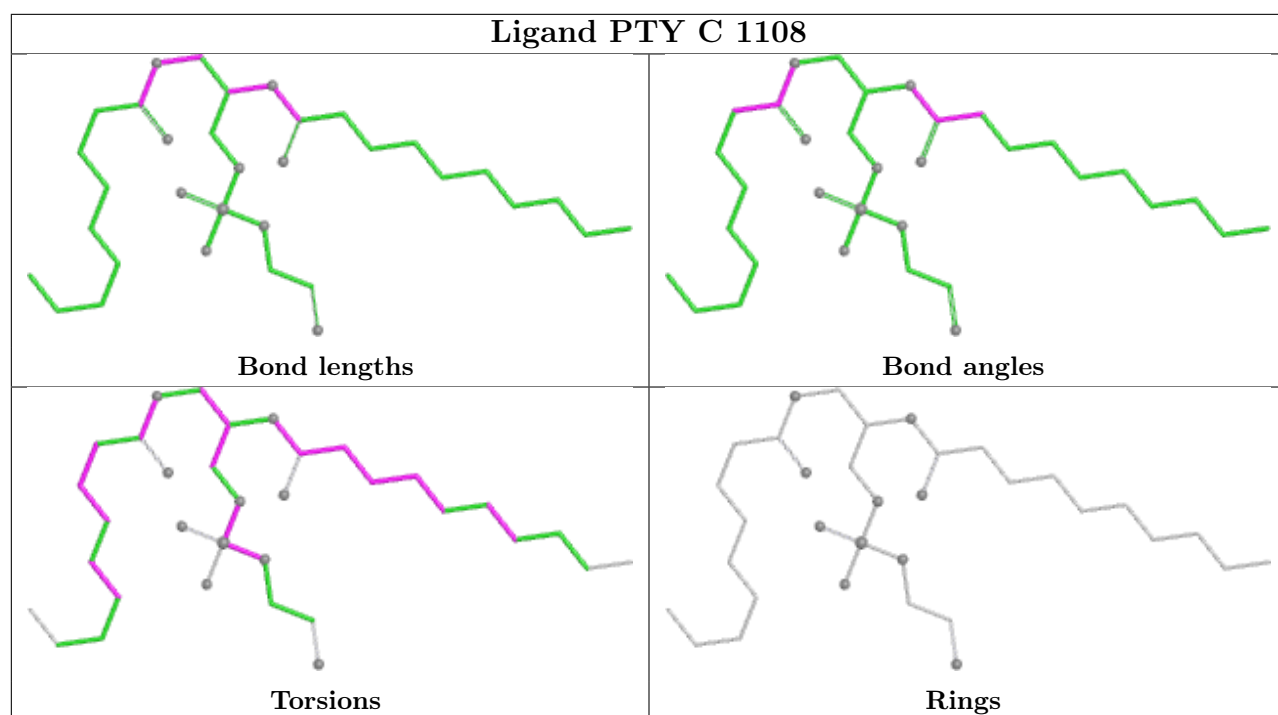
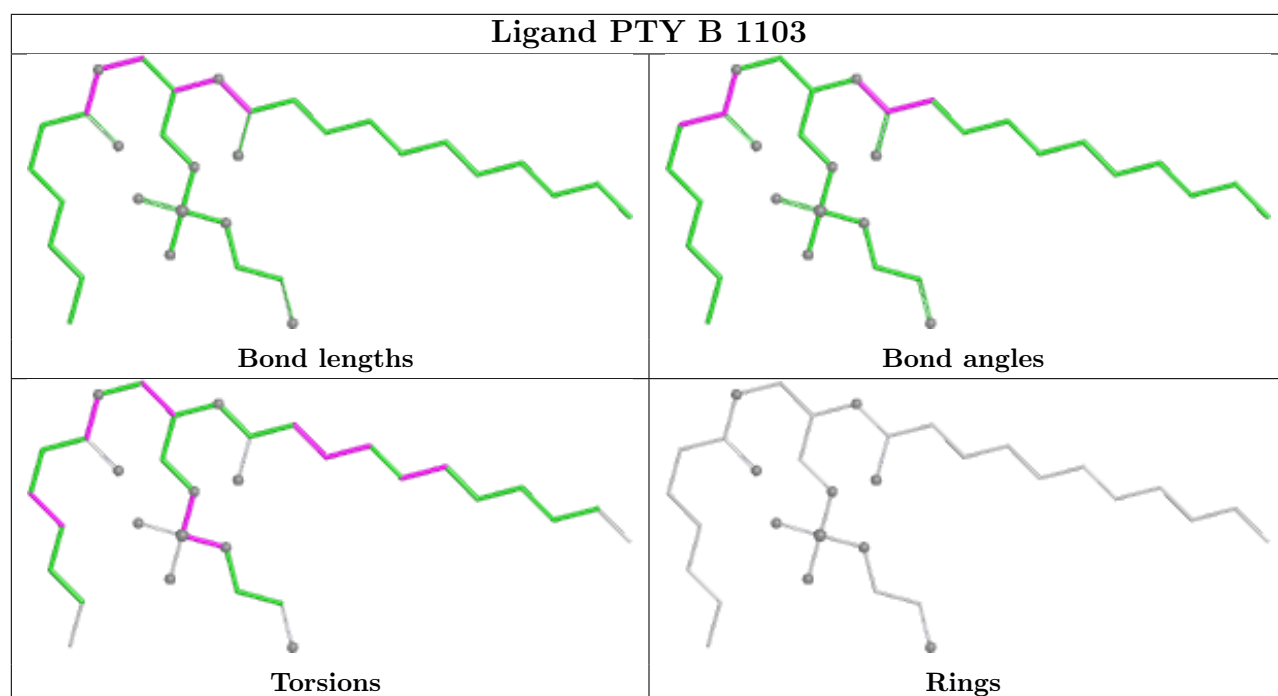
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	PTY	1	0
2	B	1109	PTY	1	0
2	B	1104	PTY	1	0
3	B	1114	D12	3	0
2	C	1106	PTY	2	0
2	A	1103	PTY	2	0

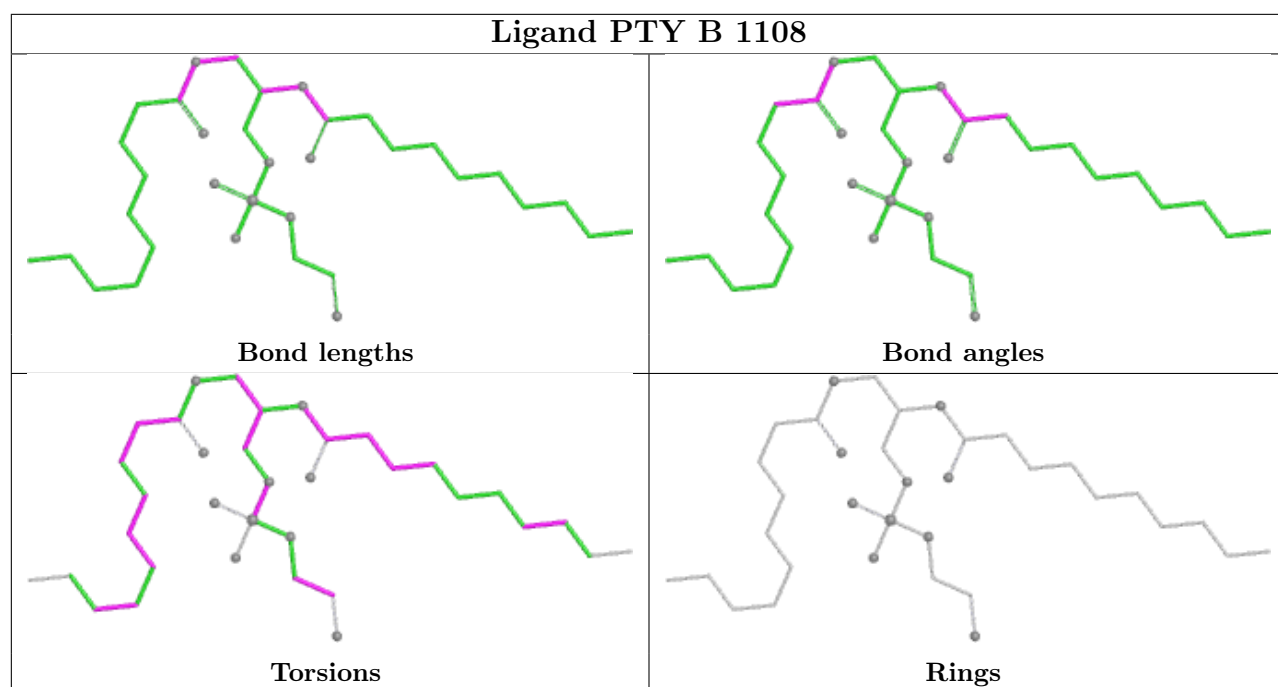
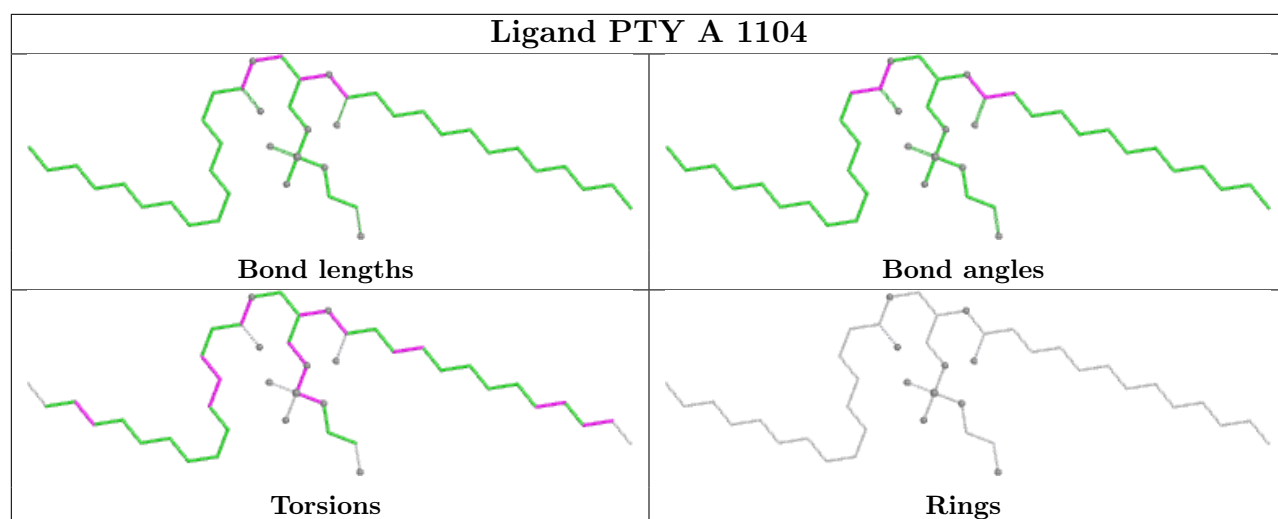
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

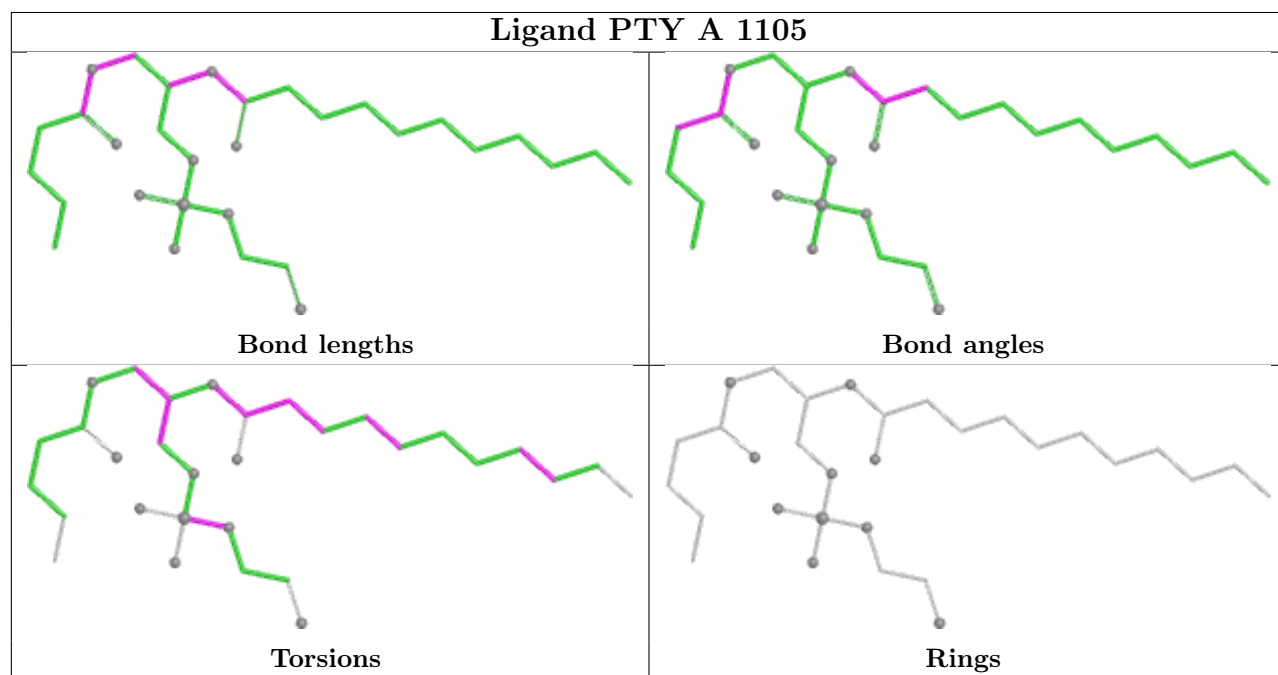
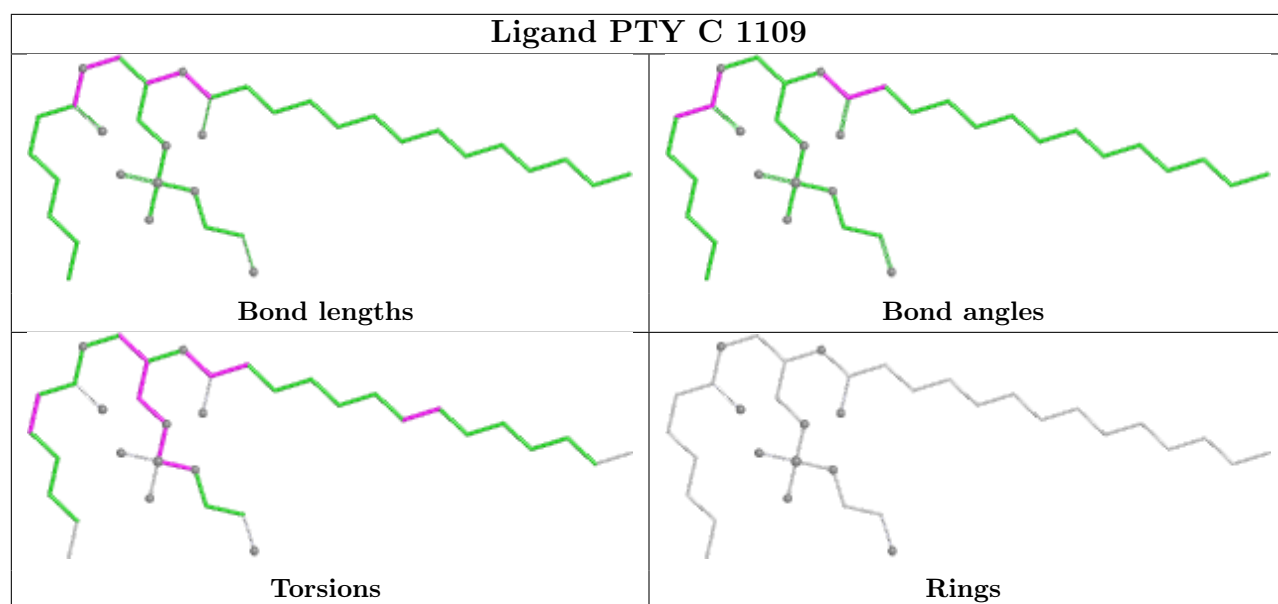


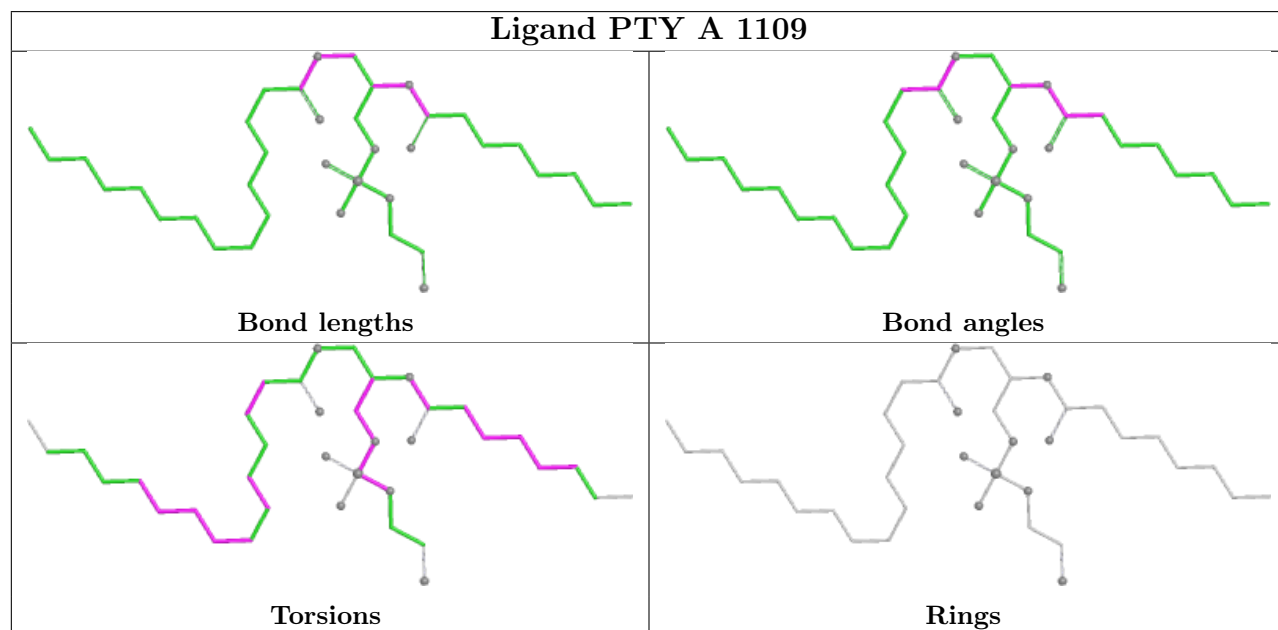
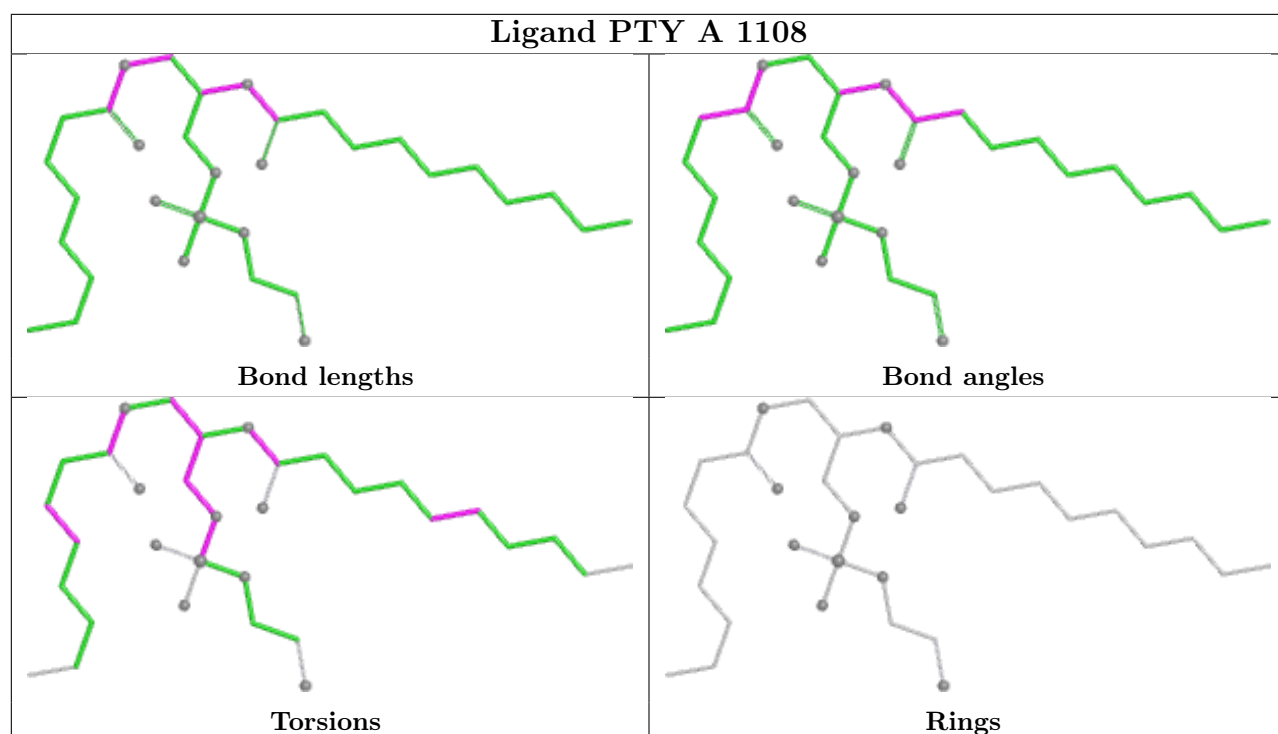


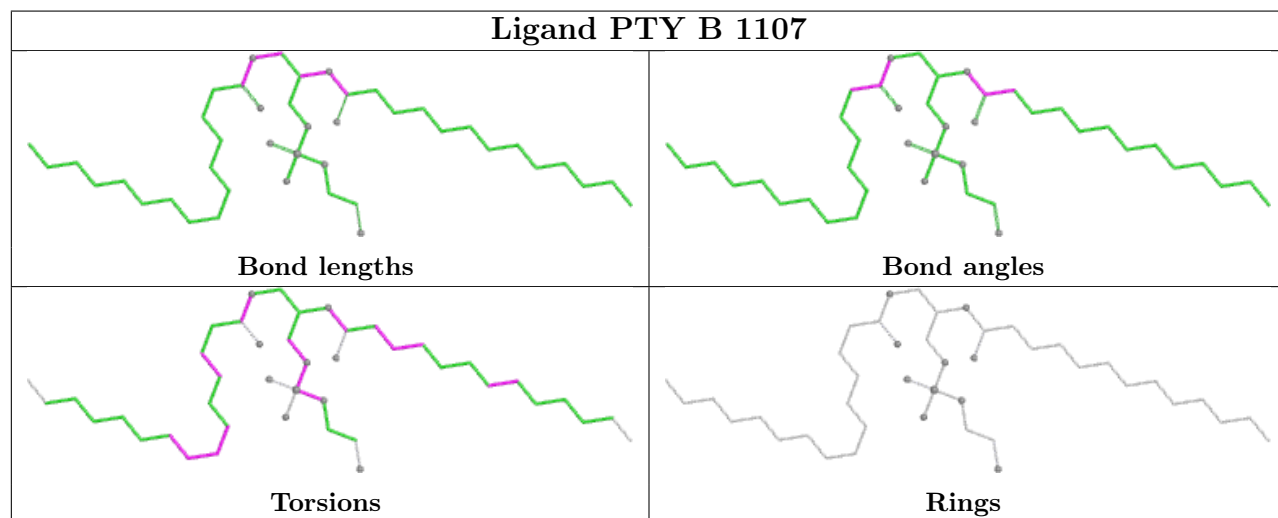
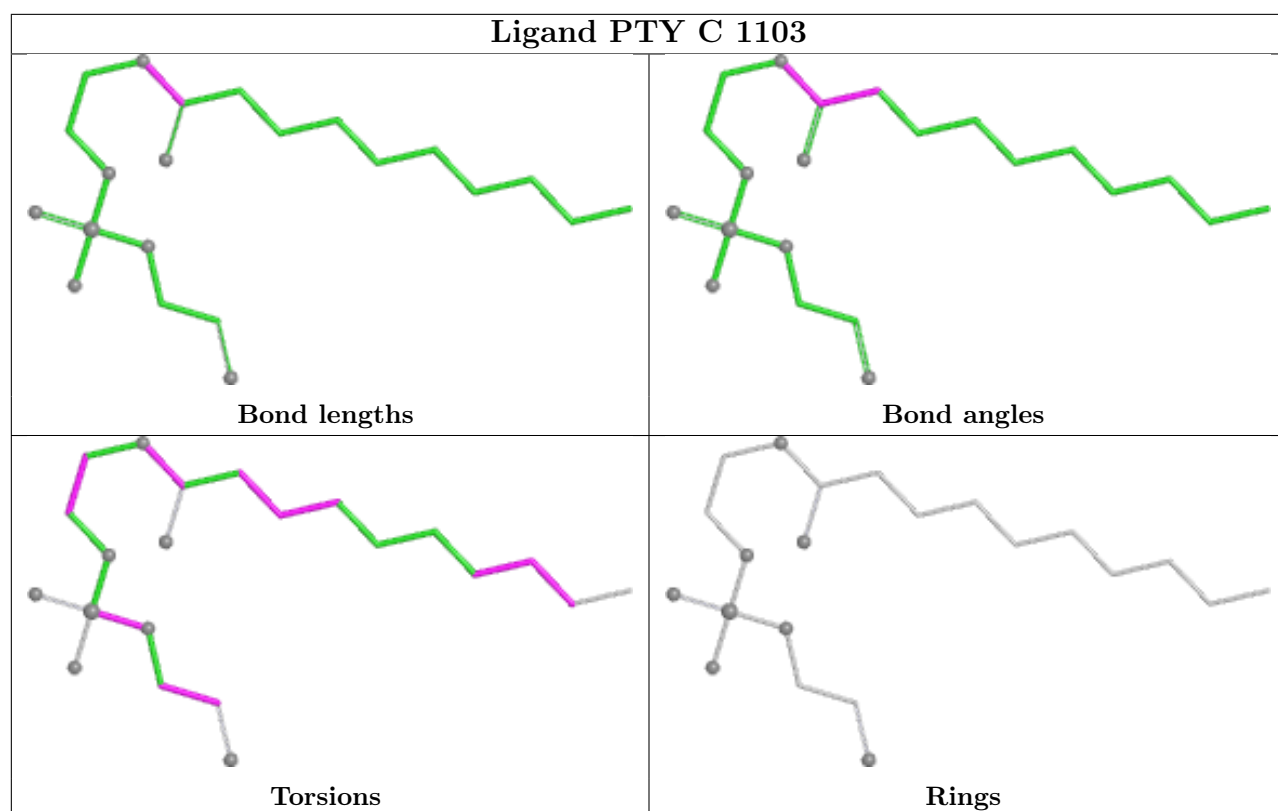


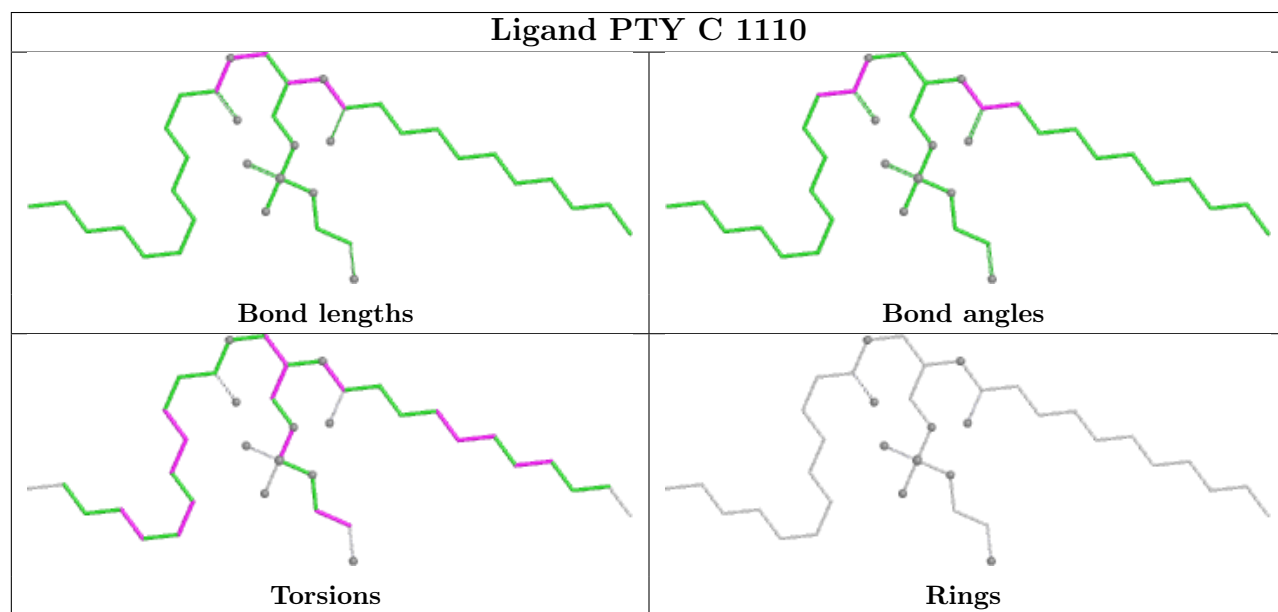
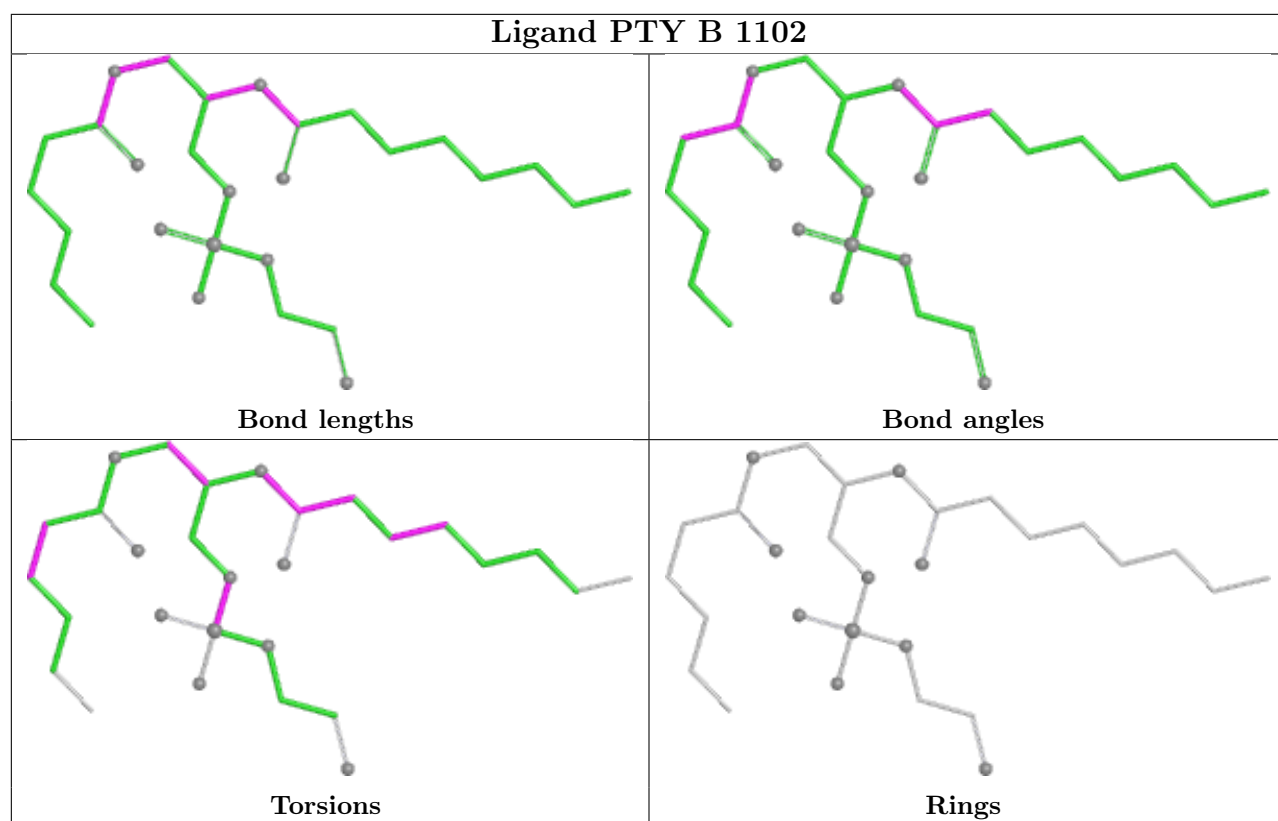


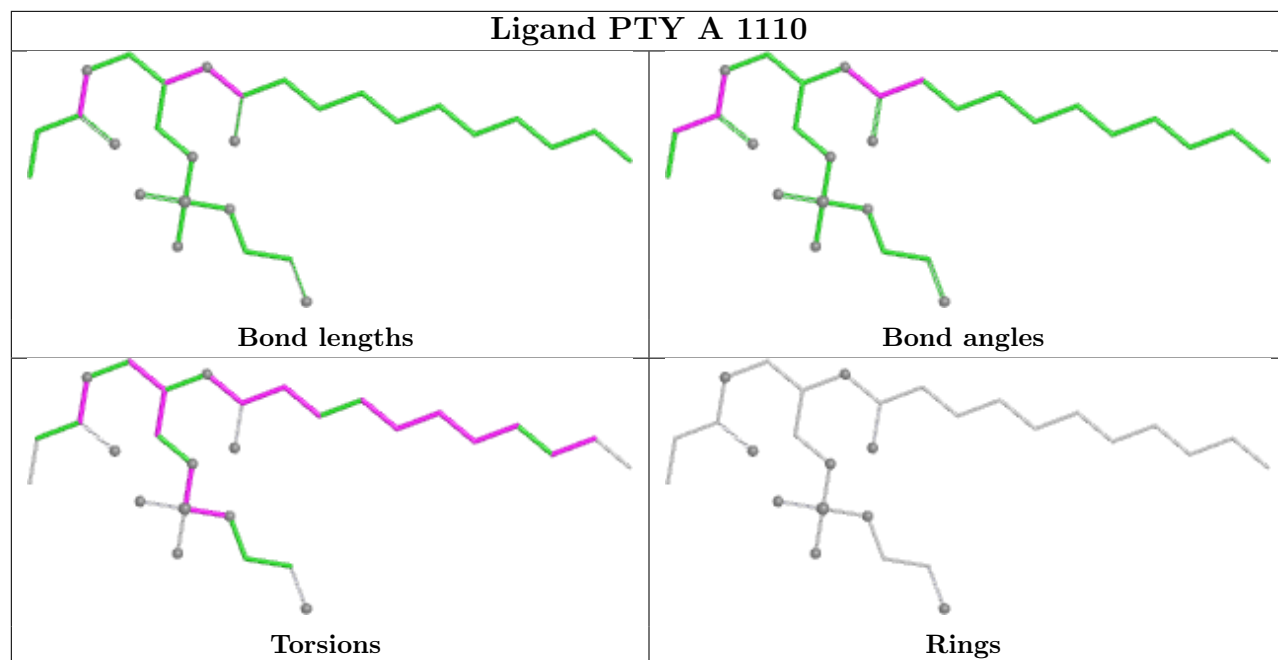


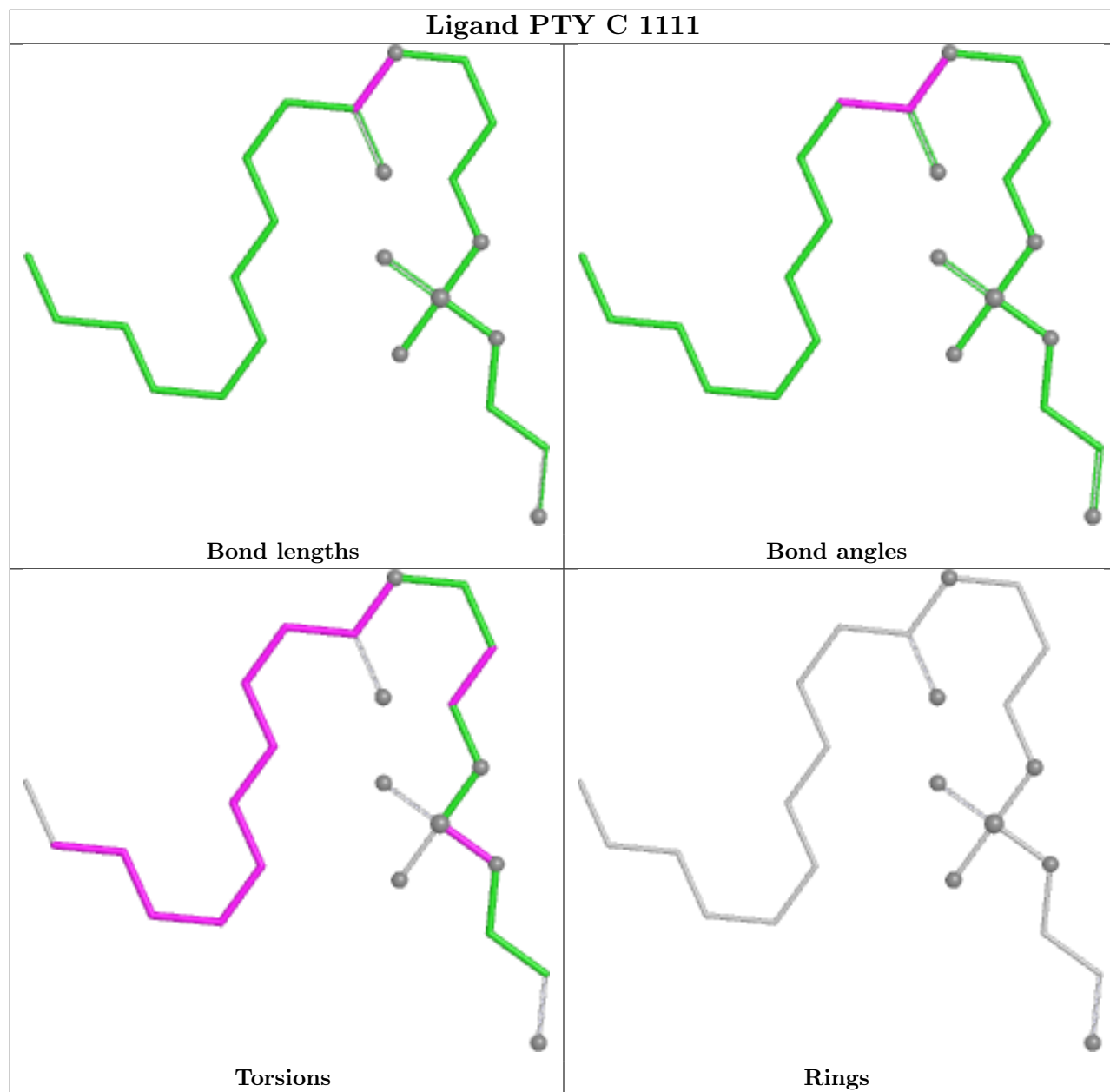


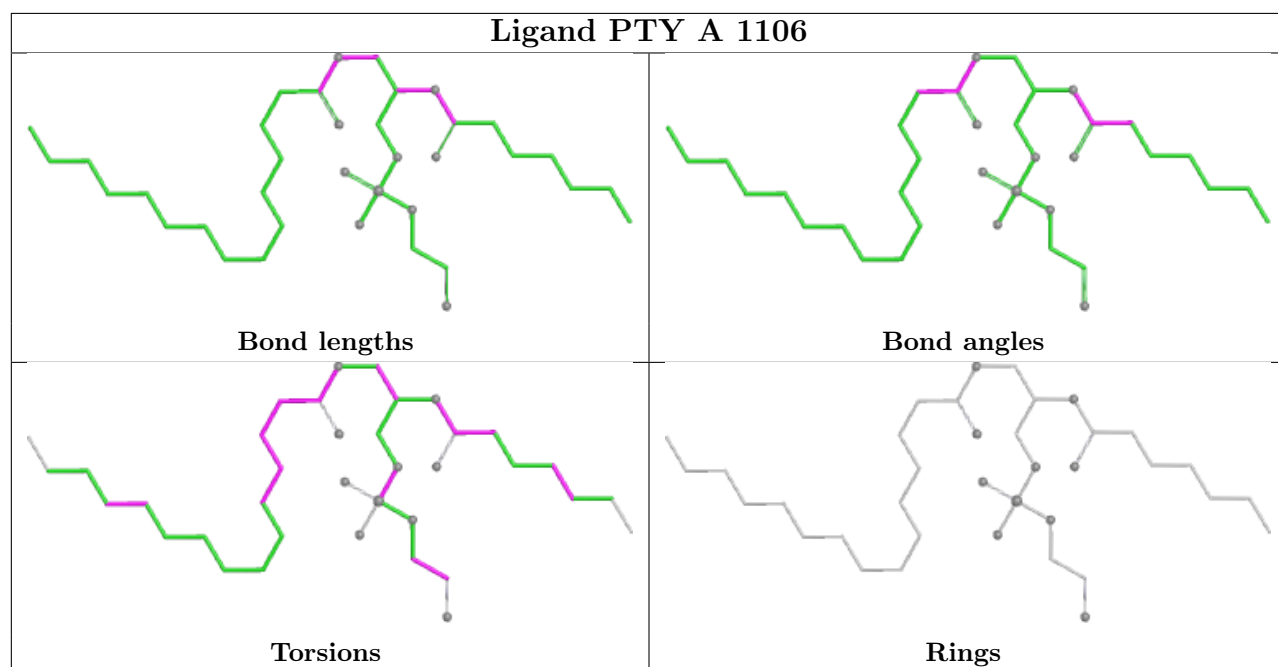
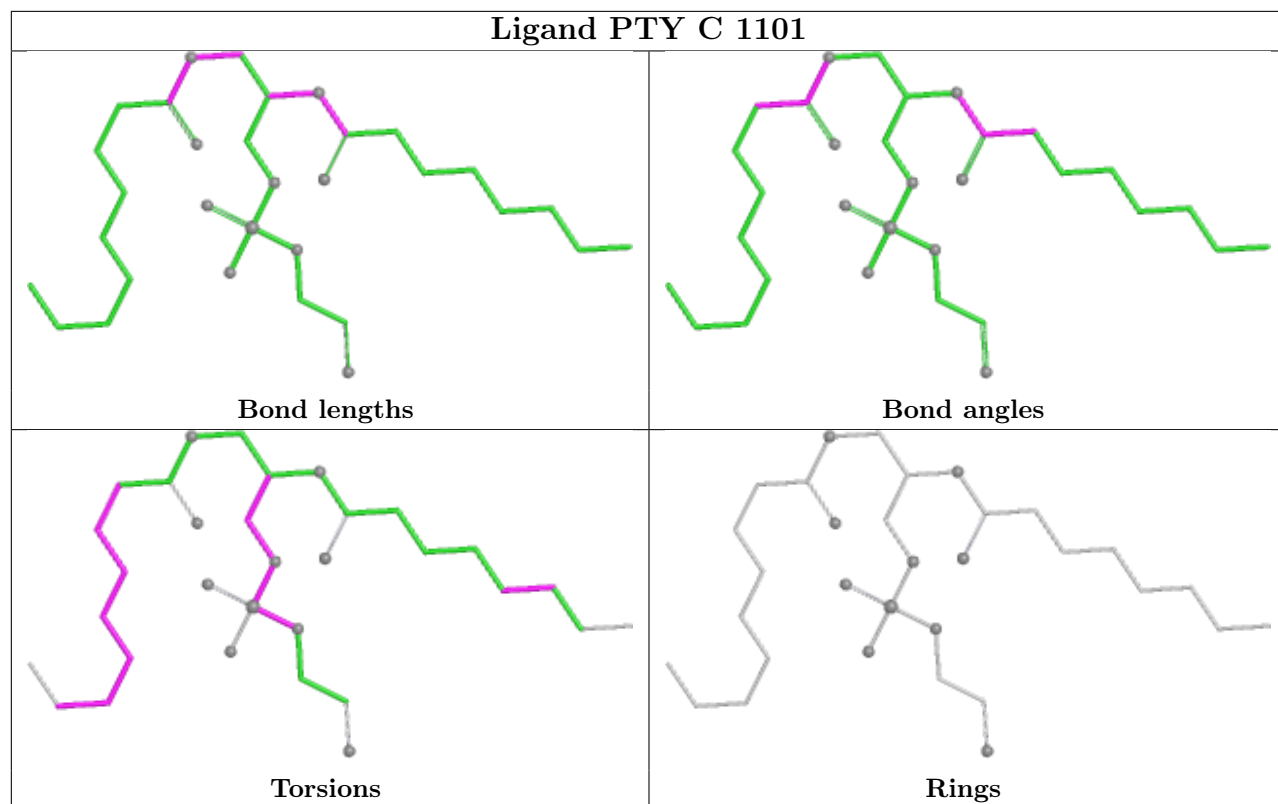


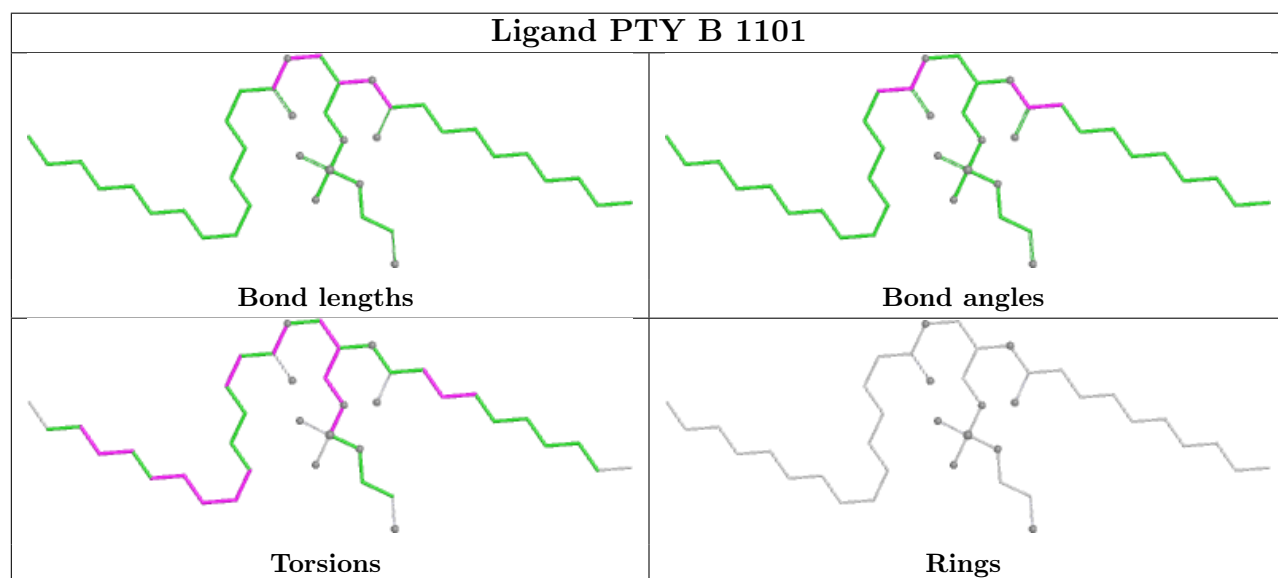
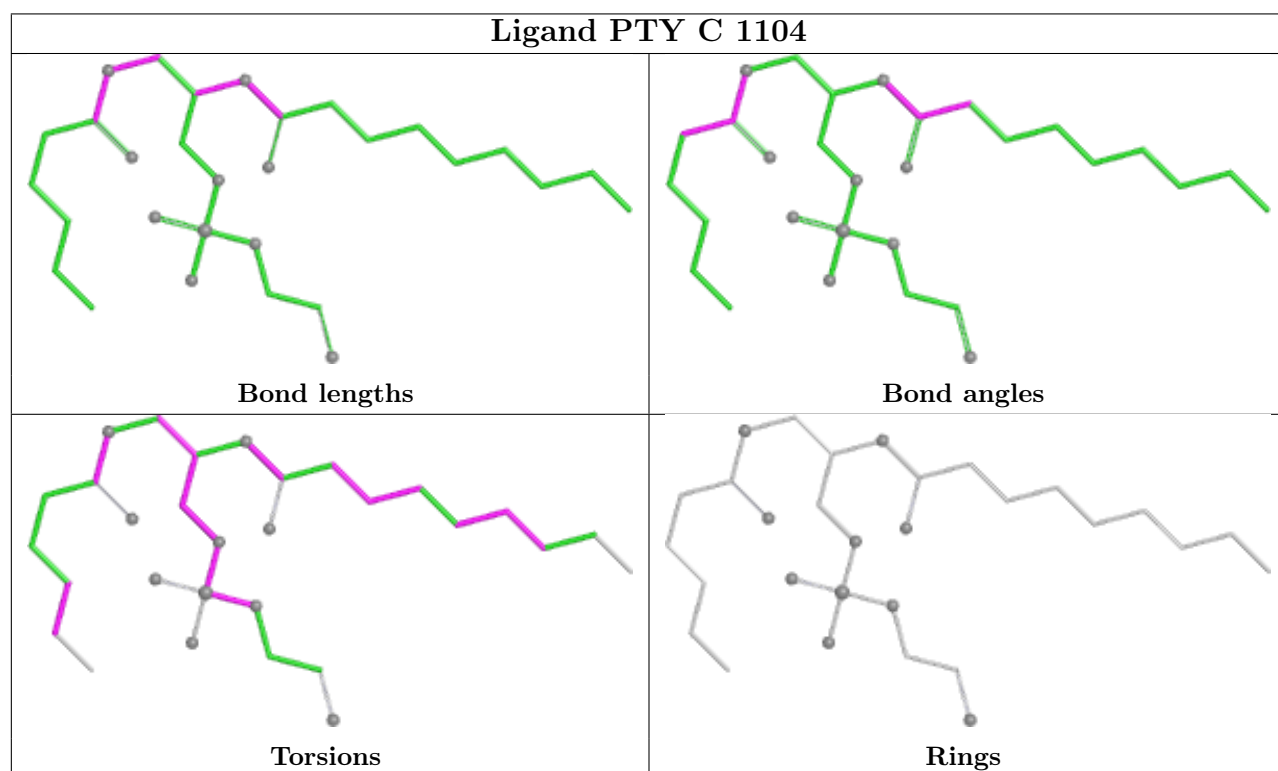
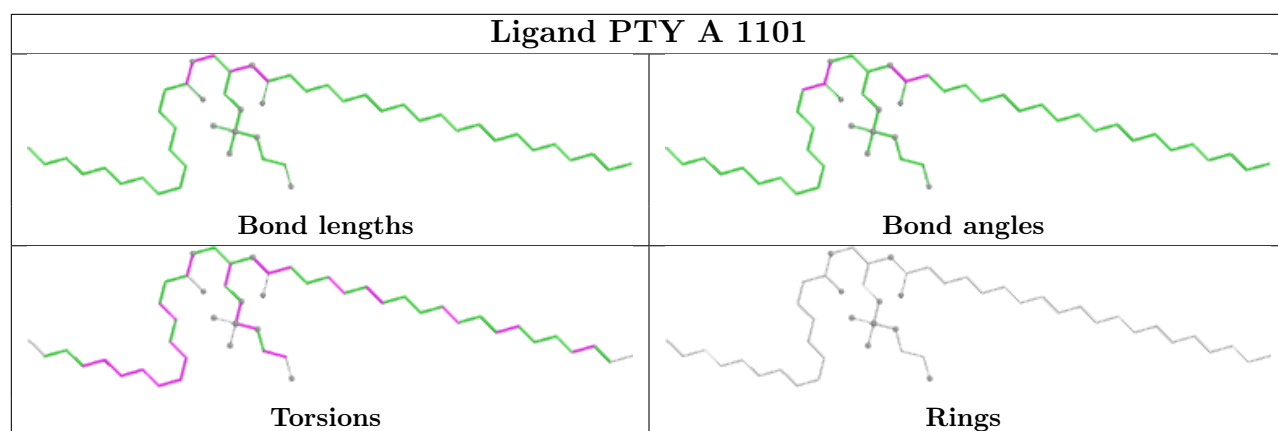


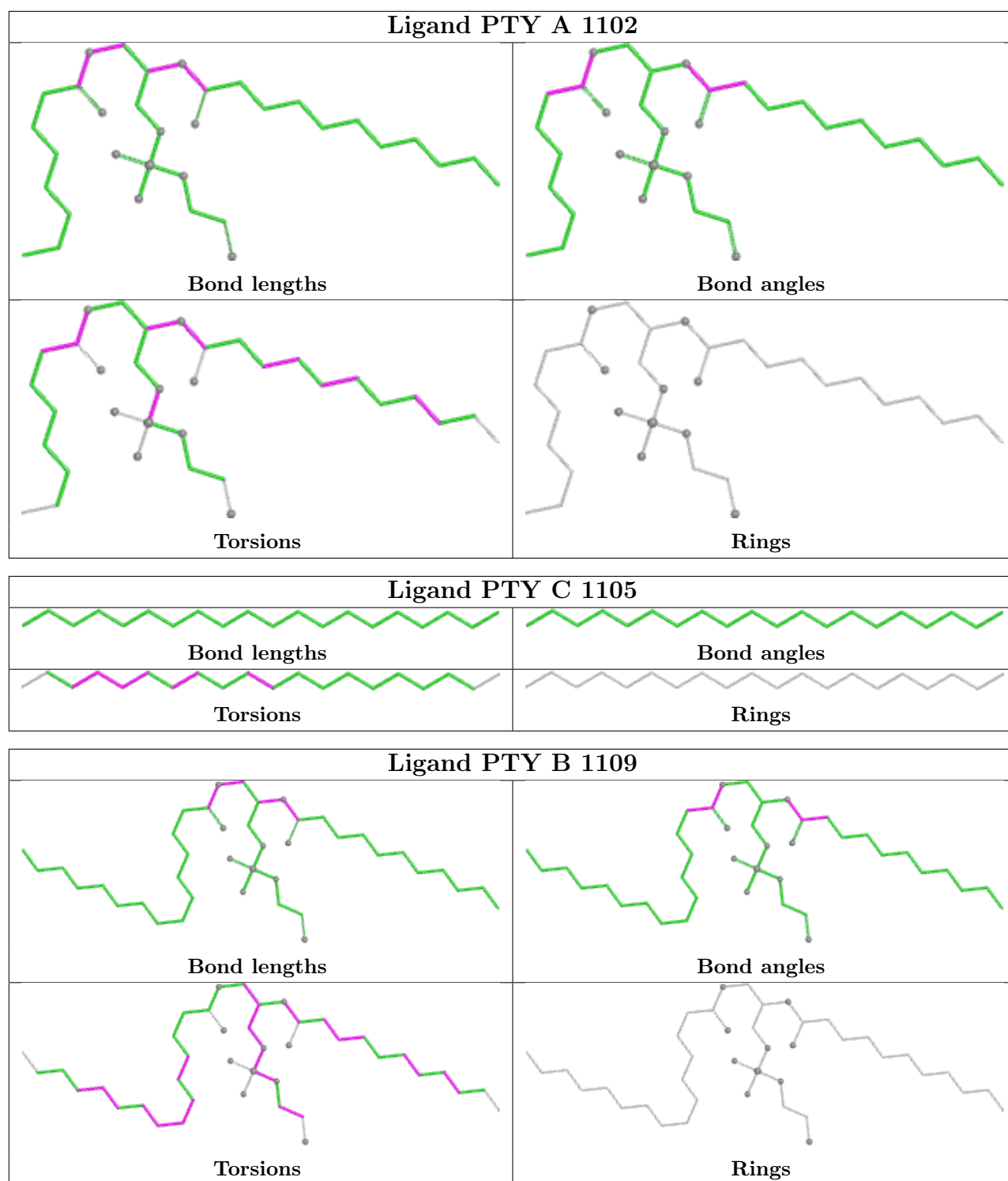


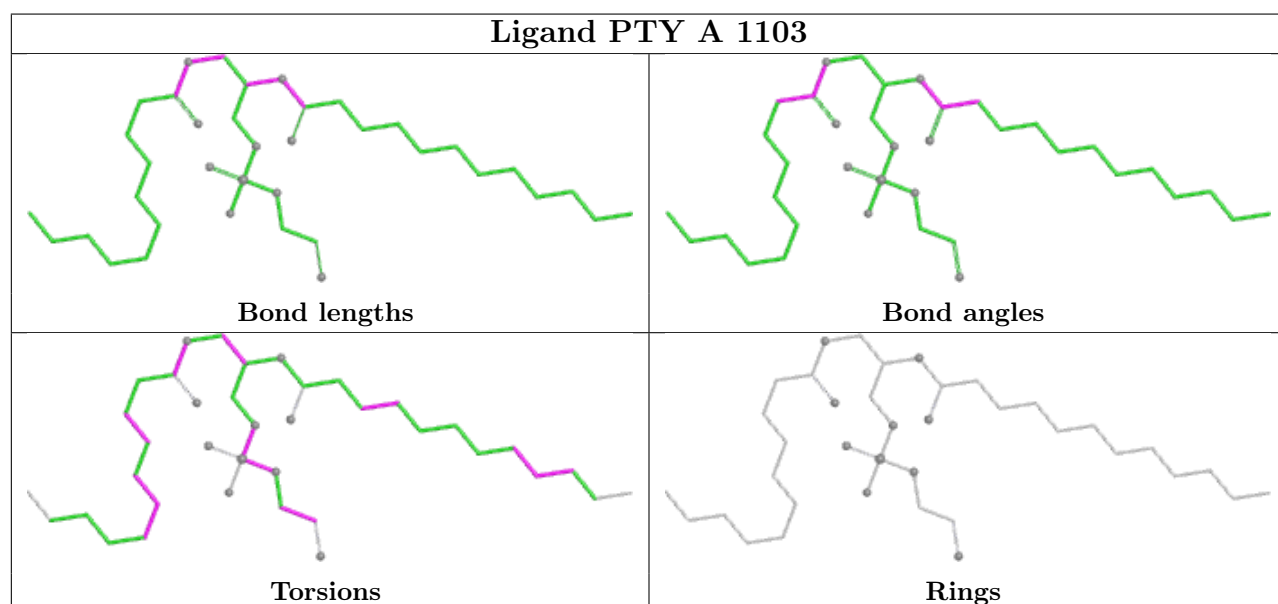
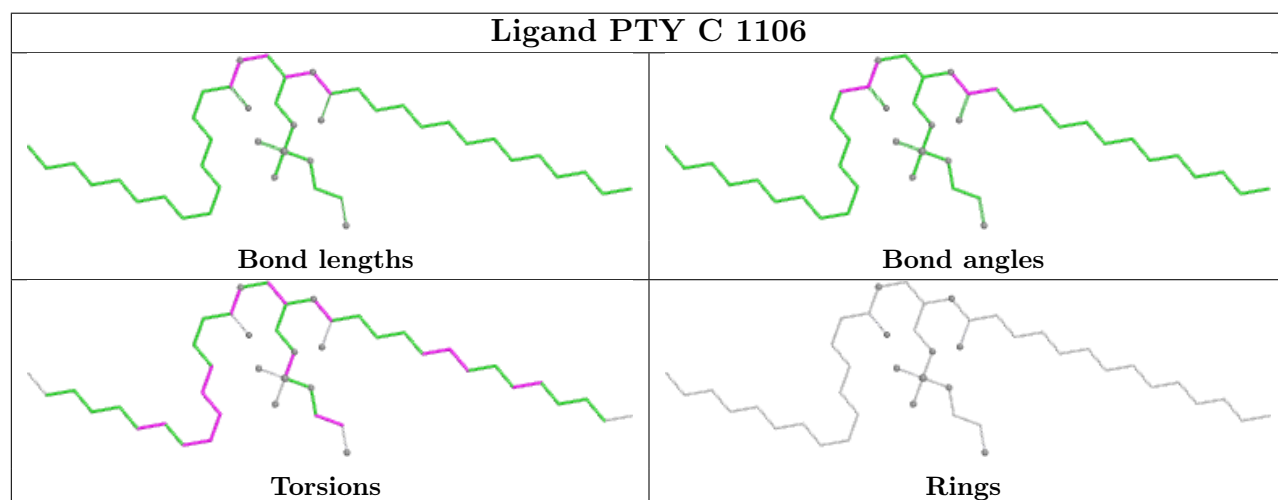
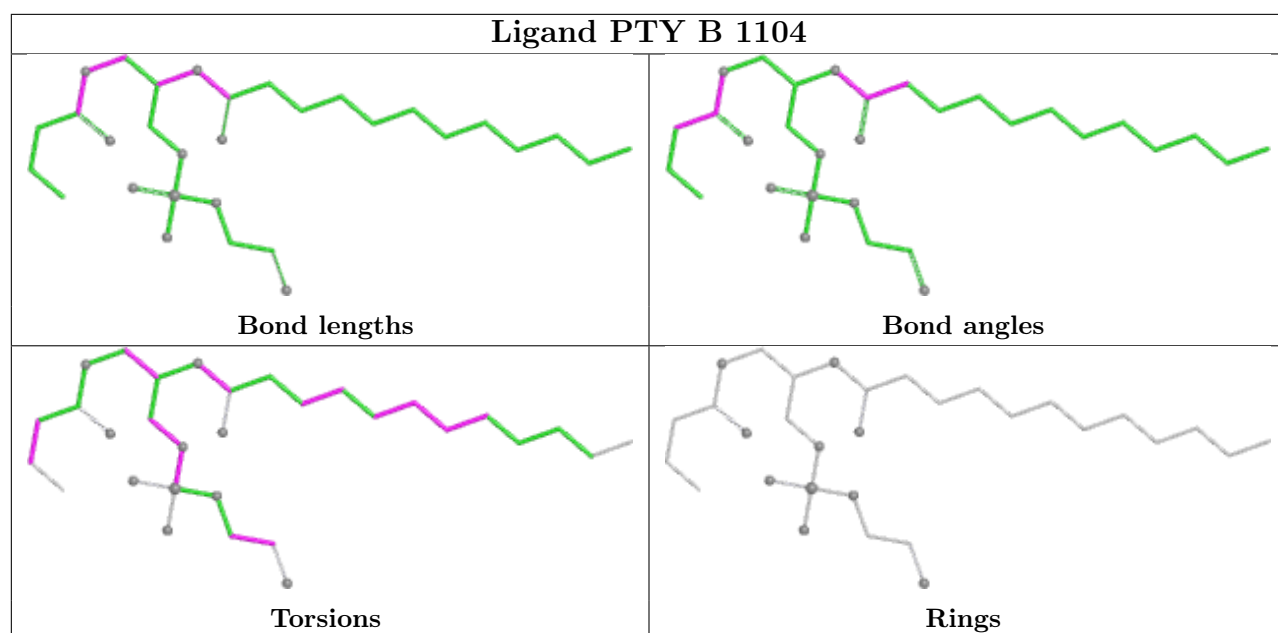












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

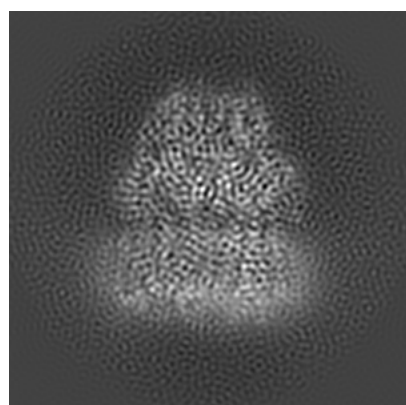
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7074. These allow visual inspection of the internal detail of the map and identification of artifacts.

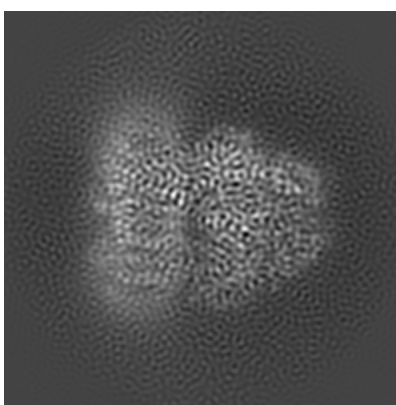
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

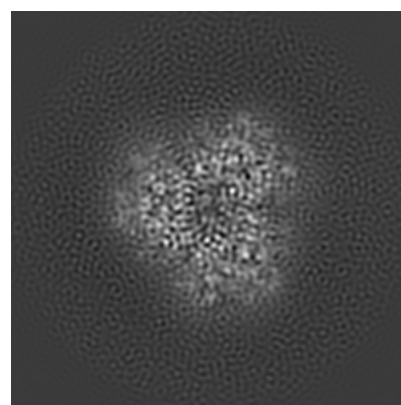
6.1.1 Primary map



X



Y

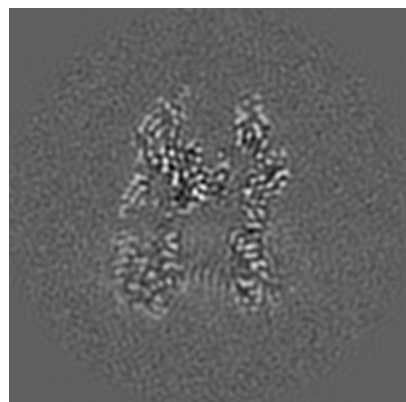


Z

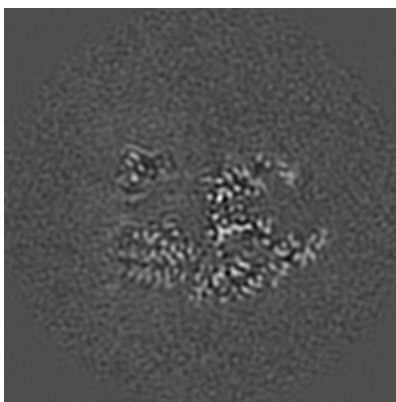
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

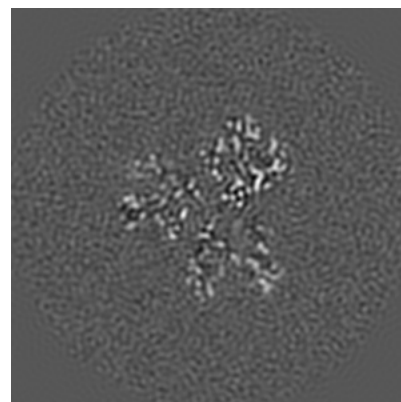
6.2.1 Primary map



X Index: 96



Y Index: 96

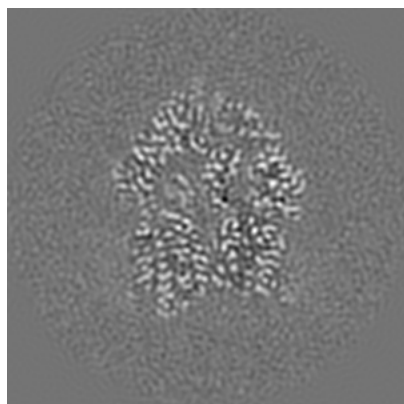


Z Index: 96

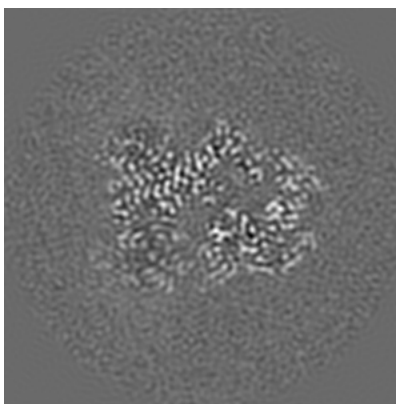
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

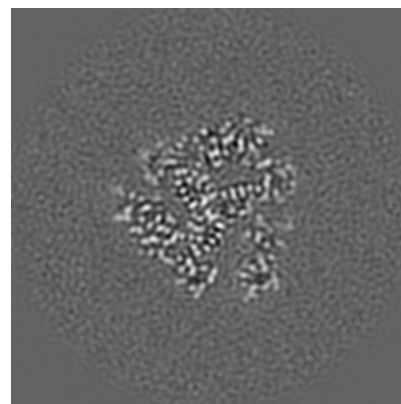
6.3.1 Primary map



X Index: 113



Y Index: 110

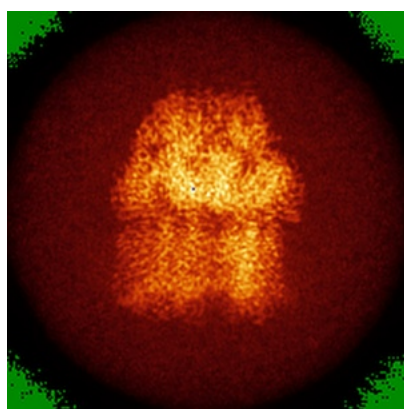


Z Index: 110

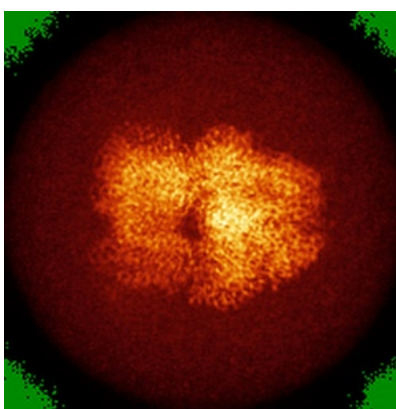
The images above show the largest variance slices of the map in three orthogonal directions.

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

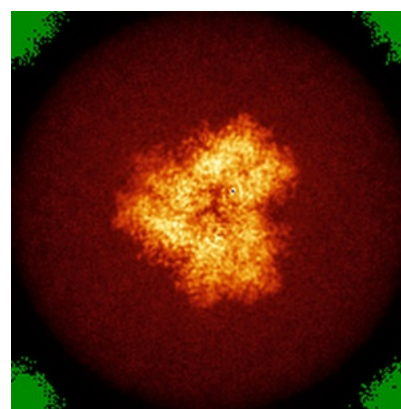
6.4.1 Primary map



X



Y

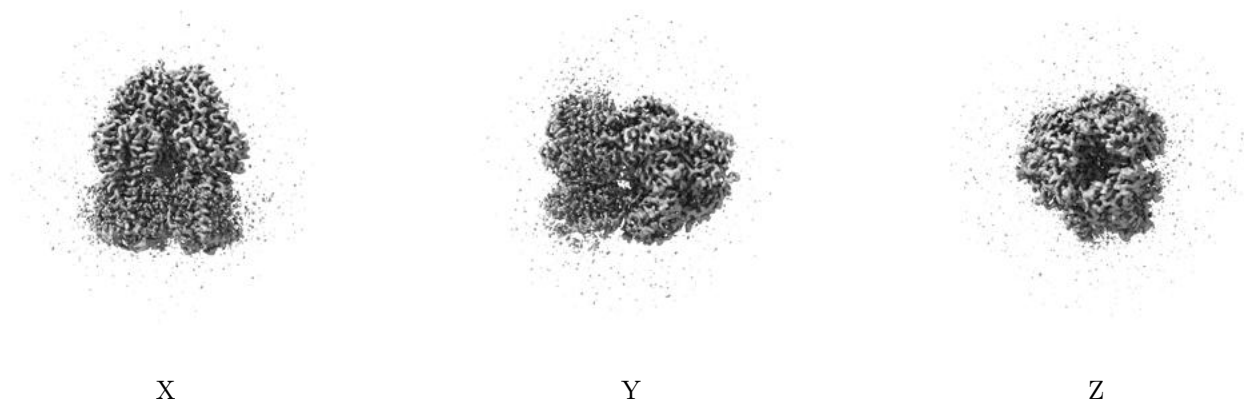


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

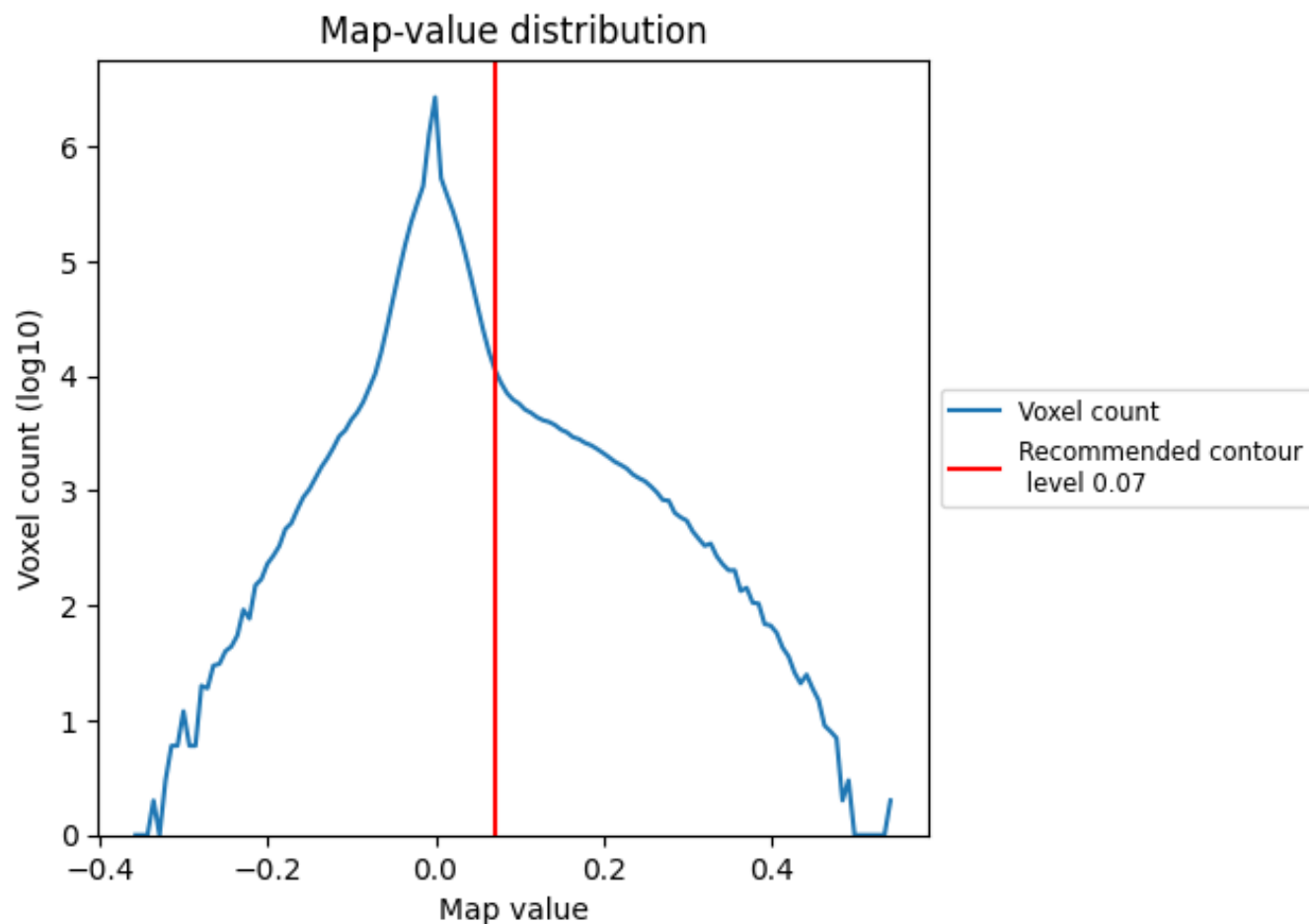
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

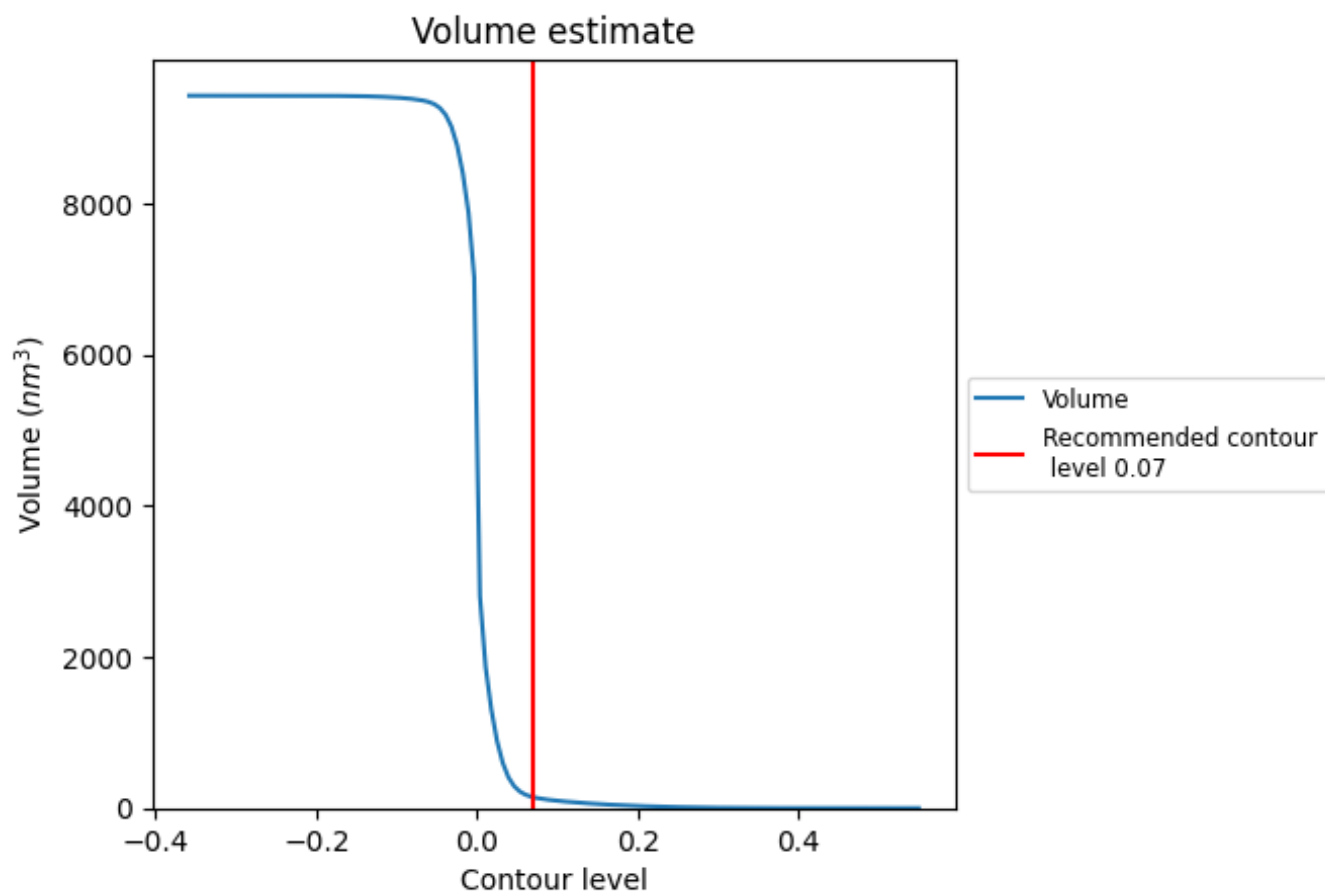
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

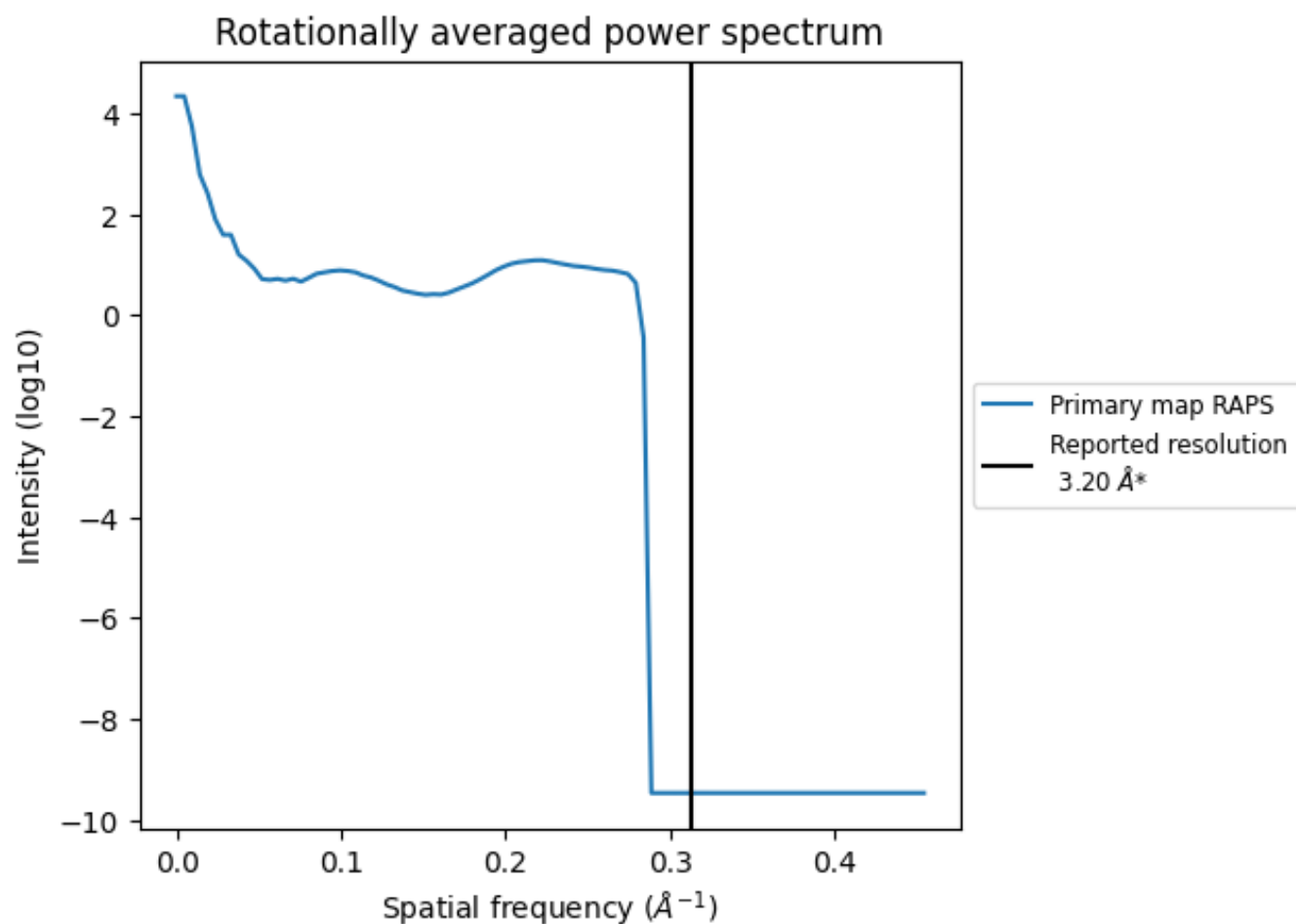
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

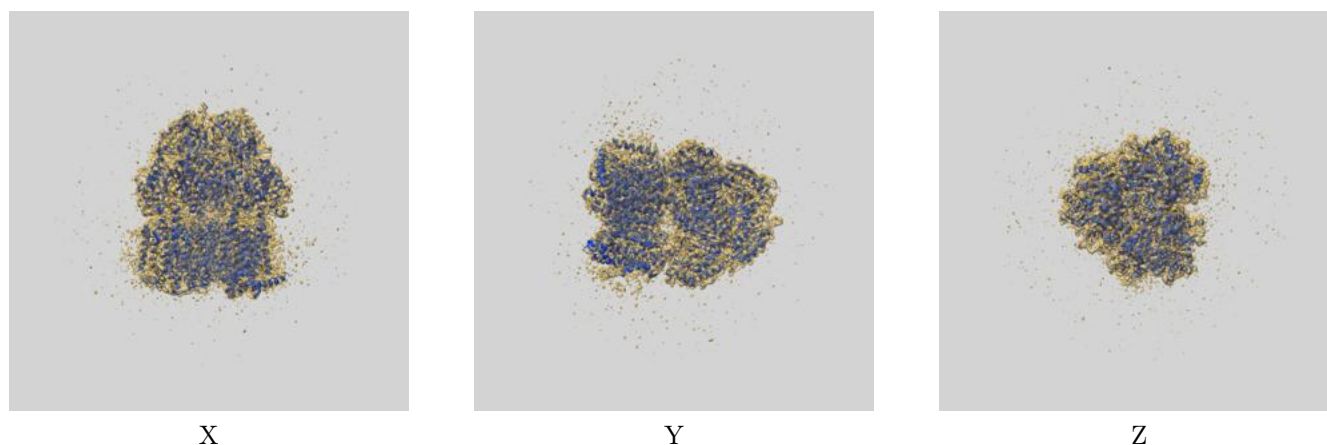
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

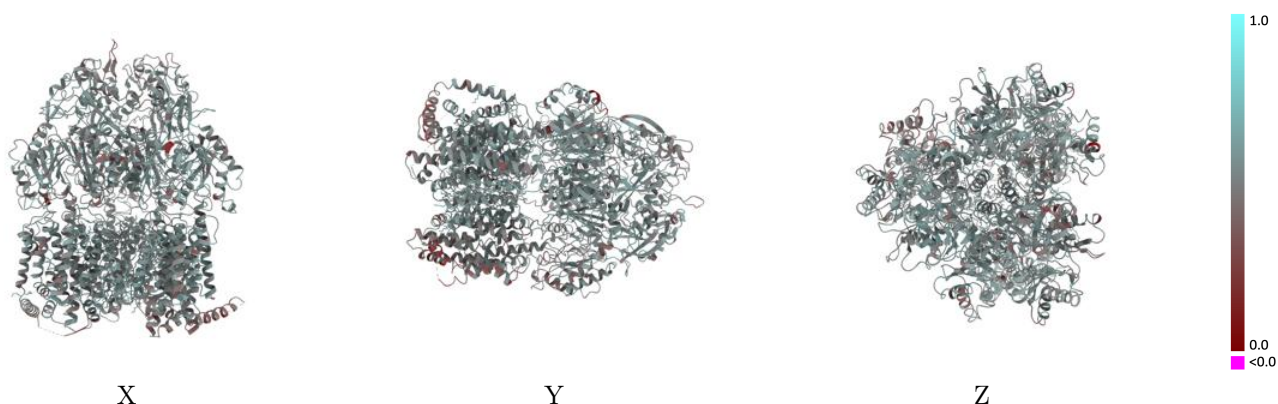
This section contains information regarding the fit between EMDB map EMD-7074 and PDB model 6BAJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



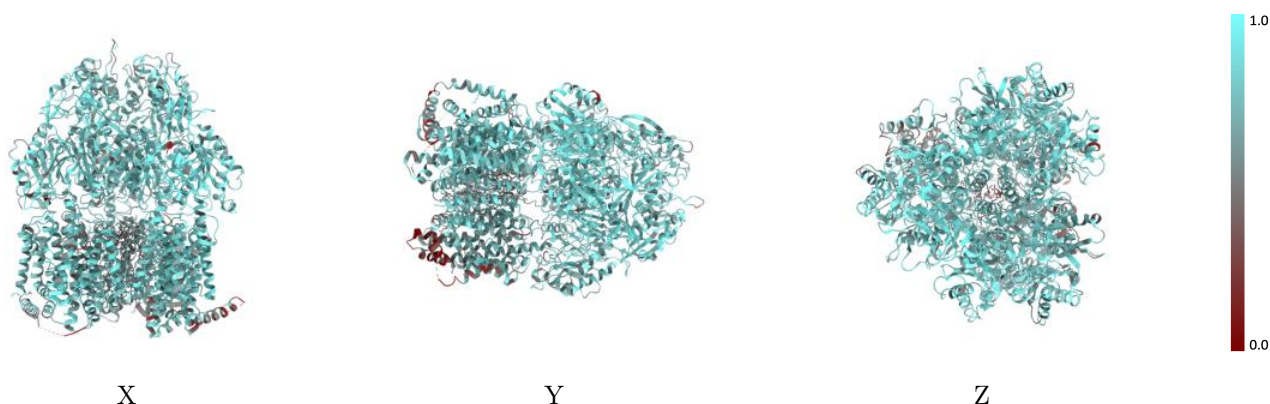
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



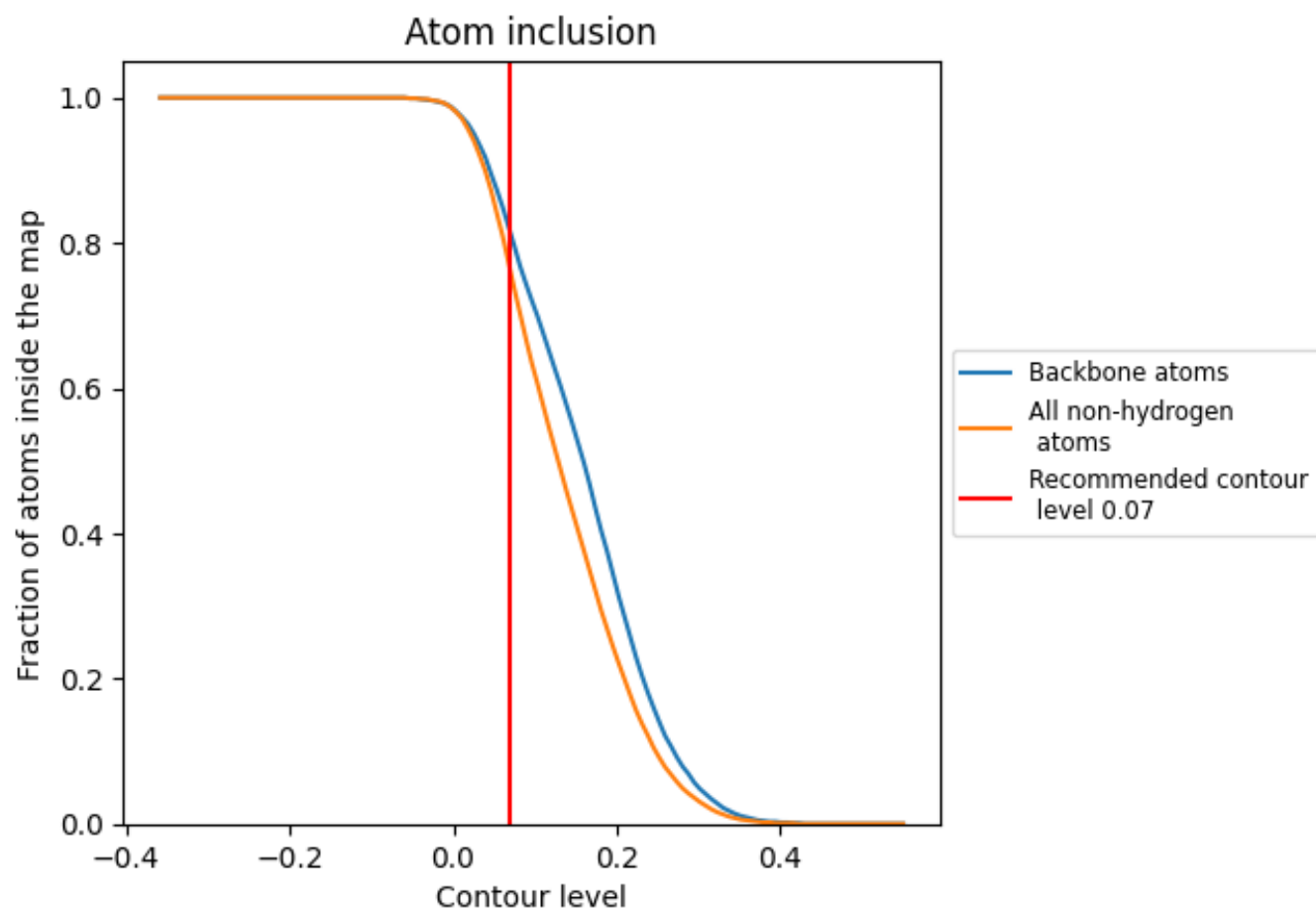
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5130
A	0.7330	0.5030
B	0.7620	0.5140
C	0.7970	0.5220

