



Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 11:16 AM JST

PDB ID : 7VD2 / pdb_00007vd2
EMDB ID : EMD-31904
Title : Human TOM complex without cross-linking
Authors : Liu, D.S.; Sui, S.F.
Deposited on : 2021-09-06
Resolution : 2.53 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:

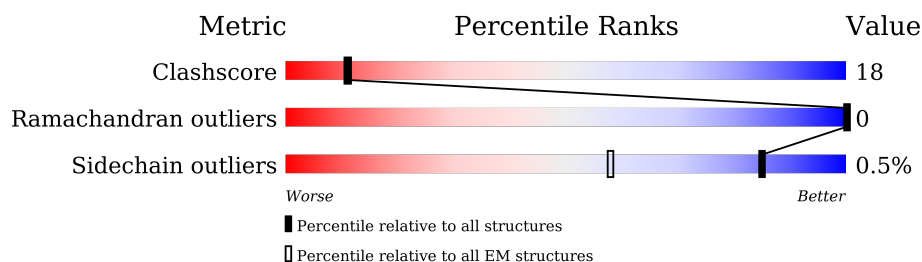
EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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 2.53 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	74	<div> <div>14%</div> <div>34%</div> <div>24%</div> <div>42%</div> </div>
1	F	74	<div> <div>14%</div> <div>35%</div> <div>23%</div> <div>42%</div> </div>
2	D	51	<div> <div>22%</div> <div>45%</div> <div>25%</div> <div>29%</div> </div>
2	E	51	<div> <div>20%</div> <div>47%</div> <div>24%</div> <div>29%</div> </div>
3	G	55	<div> <div>18%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>
3	J	55	<div> <div>18%</div> <div>56%</div> <div>42%</div> <div>.</div> </div>
4	C	142	<div> <div>11%</div> <div>23%</div> <div>18%</div> <div>60%</div> </div>
4	H	142	<div> <div>12%</div> <div>25%</div> <div>14%</div> <div>61%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	361	
5	I	361	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PC1	G	104	-	-	X	-
7	PC1	J	104	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9117 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 Mitochondrial import receptor subunit TOM6 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	43	Total	C	N	O	0	0
			354	227	67	60		
1	F	43	Total	C	N	O	0	0
			354	227	67	60		

- Molecule 2 is a protein called Mitochondrial import receptor subunit TOM5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	36	Total	C	N	O	S	0	0
			304	200	53	49	2		
2	E	36	Total	C	N	O	S	0	0
			304	200	53	49	2		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	54	Total	C	N	O	S	0	0
			433	289	74	69	1		
3	J	54	Total	C	N	O	S	0	0
			433	289	74	69	1		

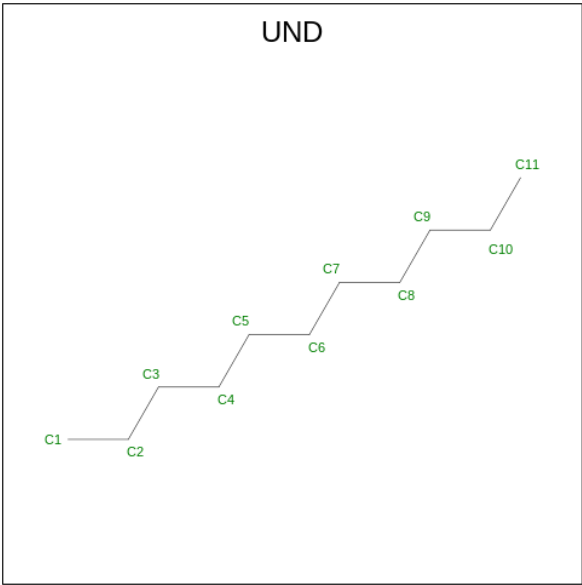
- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	56	Total	C	N	O	S	0	0
			458	297	77	81	3		
4	C	57	Total	C	N	O	S	0	0
			463	300	78	82	3		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM40 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	286	Total	C	N	O	S	0	0
			2190	1393	376	410	11		
5	I	286	Total	C	N	O	S	0	0
			2190	1393	376	410	11		

- Molecule 6 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄) (labeled as "Ligand of Interest" by depositor).



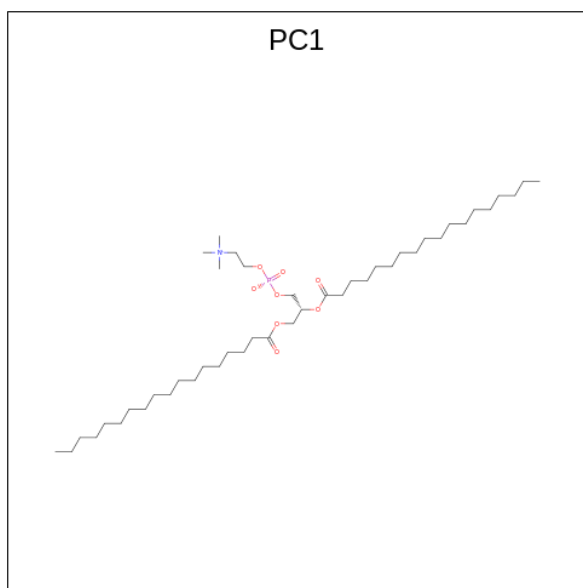
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			11	11	
6	F	1	Total	C	0
			11	11	
6	F	1	Total	C	0
			11	11	
6	G	1	Total	C	0
			11	11	
6	H	1	Total	C	0
			11	11	
6	C	1	Total	C	0
			11	11	
6	J	1	Total	C	0
			11	11	
6	B	1	Total	C	0
			11	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C 11 11	0
6	B	1	Total C 11 11	0
6	B	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	I	1	Total C 11 11	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O P 54 44 1 8 1	0
7	A	1	Total C N O P 54 44 1 8 1	0
7	F	1	Total C N O P 54 44 1 8 1	0
7	G	1	Total C N O P 54 44 1 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	J	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	J	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	J	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	J	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	

Continued on next page...

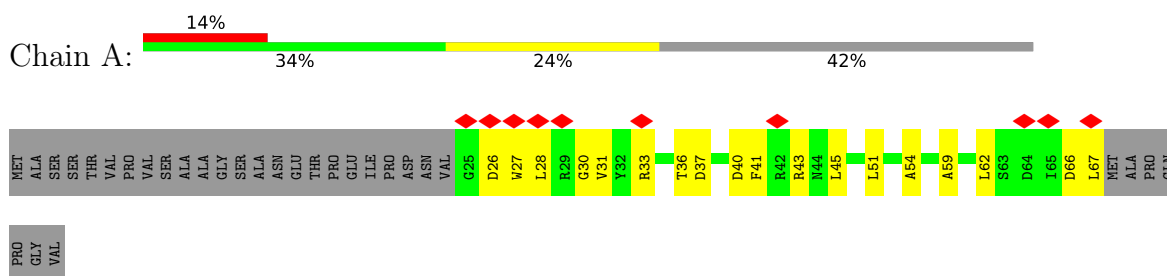
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	

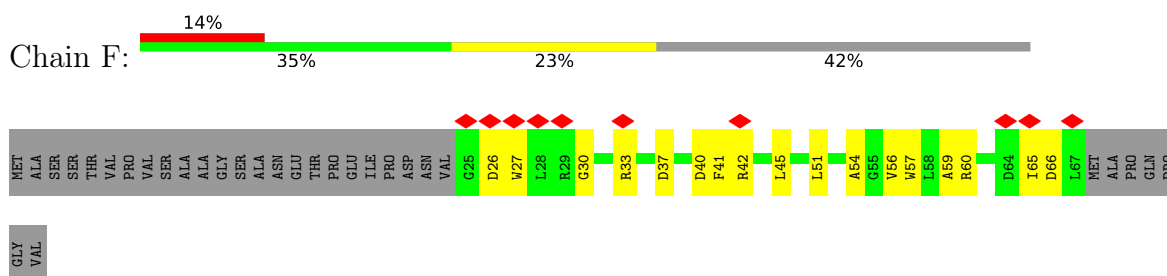
3 Residue-property plots [i](#)

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.

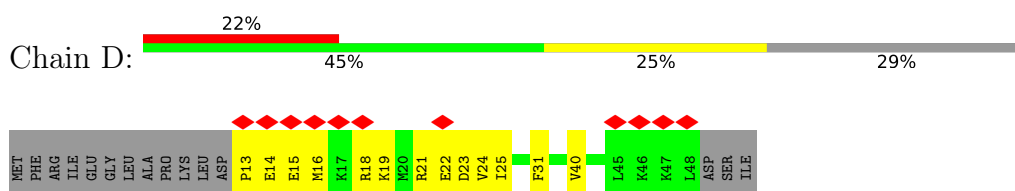
- Molecule 1: Mitochondrial import receptor subunit TOM6 homolog



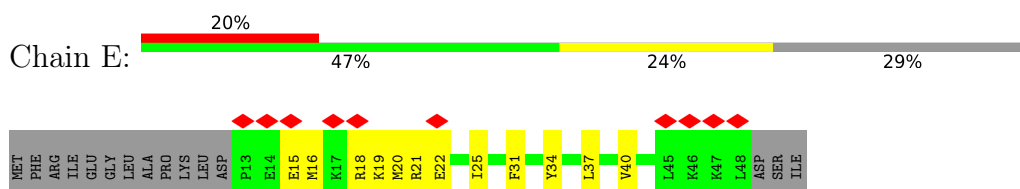
- Molecule 1: Mitochondrial import receptor subunit TOM6 homolog



- Molecule 2: Mitochondrial import receptor subunit TOM5 homolog



- Molecule 2: Mitochondrial import receptor subunit TOM5 homolog



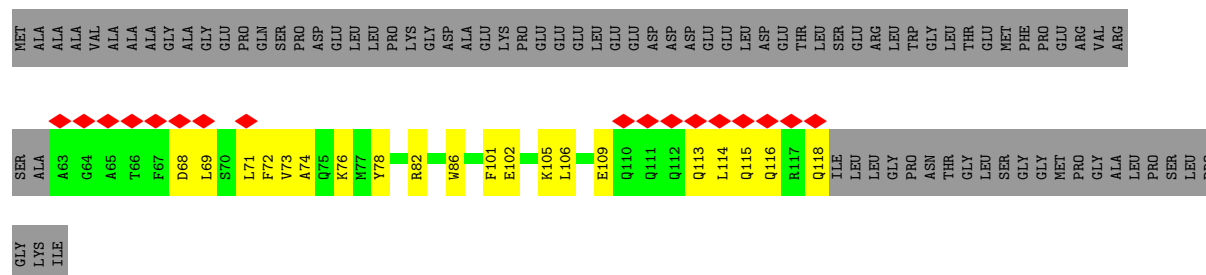
- Molecule 3: Mitochondrial import receptor subunit TOM7 homolog



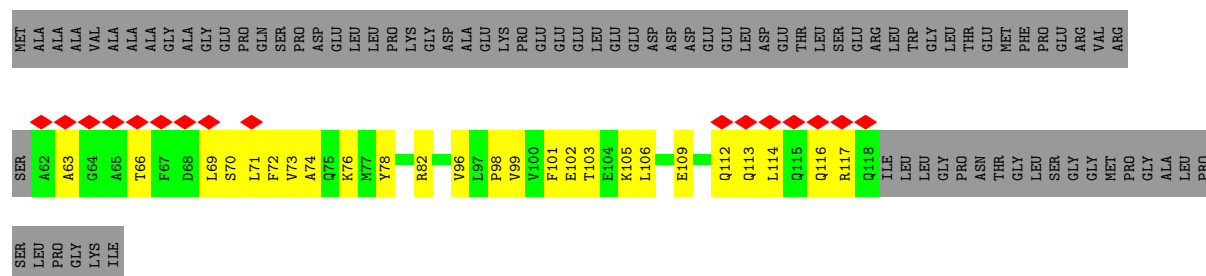
- Chain J:  18% 56% 42%



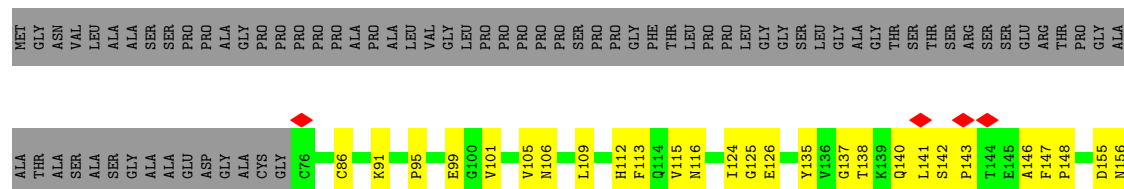
- Chain H: 

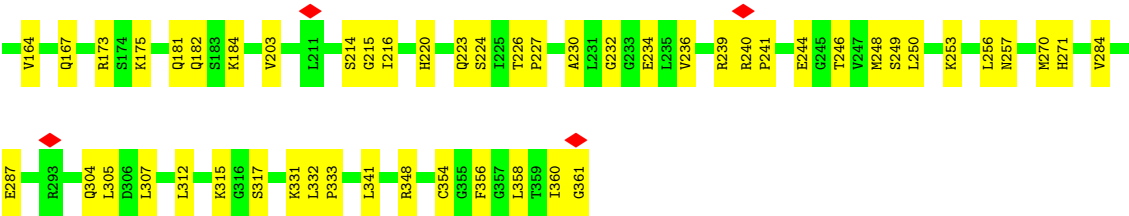


- Chain C: 

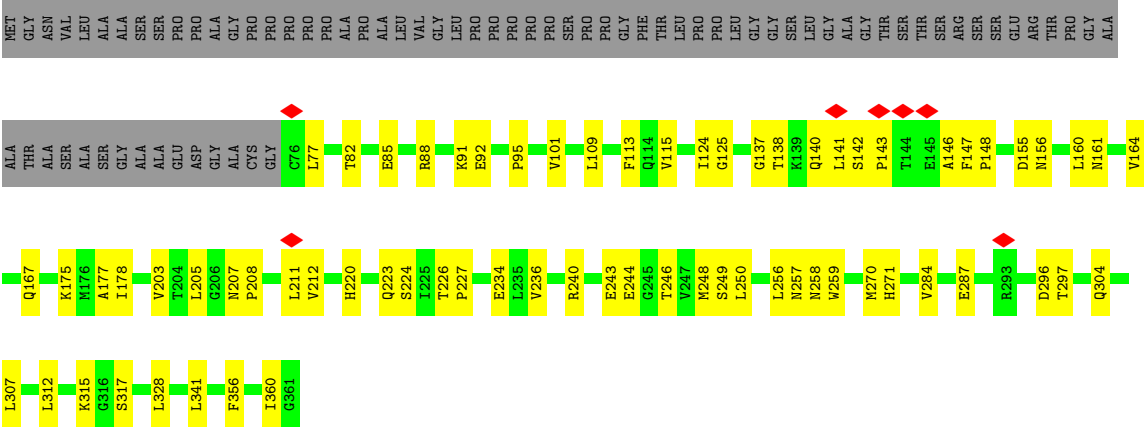


- Chain B: 





• Molecule 5: Mitochondrial import receptor subunit TOM40 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	347651	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.107	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	269.856, 269.856, 269.856	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8433, 0.8433, 0.8433	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, UND

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	0.33	0/361	0.35	0/488
1	F	0.34	0/361	0.34	0/488
2	D	0.29	0/308	0.37	0/410
2	E	0.30	0/308	0.40	0/410
3	G	0.37	0/445	0.37	0/599
3	J	0.35	0/445	0.35	0/599
4	C	0.35	0/471	0.34	0/634
4	H	0.34	0/466	0.33	0/627
5	B	0.47	0/2240	0.40	0/3039
5	I	0.47	0/2240	0.42	0/3039
All	All	0.42	0/7645	0.39	0/10333

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	354	0	349	20	0
1	F	354	0	349	14	0
2	D	304	0	339	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	304	0	339	17	0
3	G	433	0	456	37	0
3	J	433	0	456	42	0
4	C	463	0	470	25	0
4	H	458	0	465	21	0
5	B	2190	0	2171	72	0
5	I	2190	0	2171	73	0
6	A	22	0	48	0	0
6	B	44	0	96	7	0
6	C	11	0	24	0	0
6	F	22	0	48	0	0
6	G	11	0	24	0	0
6	H	11	0	24	0	0
6	I	44	0	96	7	0
6	J	11	0	24	0	0
7	A	108	0	176	3	0
7	B	270	0	440	22	0
7	C	108	0	176	4	0
7	F	54	0	88	0	0
7	G	216	0	352	28	0
7	H	162	0	264	10	0
7	I	324	0	528	22	0
7	J	216	0	352	31	0
All	All	9117	0	10325	350	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 18.

All (350) 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)
7:J:104:PC1:H331	7:J:104:PC1:C26	1.49	1.42
7:G:104:PC1:H331	7:G:104:PC1:C26	1.49	1.40
3:J:25:TRP:CD2	7:J:104:PC1:H151	1.81	1.15
3:G:25:TRP:CD2	7:G:104:PC1:H151	1.83	1.13
7:J:104:PC1:H331	7:J:104:PC1:H261	1.18	1.12
7:J:104:PC1:H331	7:J:104:PC1:H262	1.26	1.11
7:G:104:PC1:H331	7:G:104:PC1:H262	1.26	1.11
3:G:25:TRP:CE2	7:G:104:PC1:C15	2.36	1.09
3:J:25:TRP:CE2	7:J:104:PC1:C15	2.36	1.07
7:G:104:PC1:H331	7:G:104:PC1:H261	1.18	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:LYS:HB2	3:G:9:LYS:HZ2	1.25	0.98
7:G:104:PC1:H261	7:G:104:PC1:C33	1.95	0.97
5:B:203:VAL:HG23	7:B:406:PC1:H151	1.46	0.97
7:J:104:PC1:H261	7:J:104:PC1:C33	1.95	0.96
5:B:138:THR:H	6:B:405:UND:H111	1.28	0.96
5:B:106:ASN:HB2	5:B:361:GLY:HA3	1.47	0.96
3:J:25:TRP:CE2	7:J:104:PC1:H151	1.99	0.95
7:J:104:PC1:H281	7:J:104:PC1:H351	1.48	0.95
7:G:104:PC1:H281	7:G:104:PC1:H351	1.48	0.94
7:G:104:PC1:C26	7:G:104:PC1:C33	2.45	0.93
3:G:25:TRP:CE2	7:G:104:PC1:H151	1.99	0.93
4:H:69:LEU:HD11	7:H:202:PC1:O12	1.70	0.92
5:B:203:VAL:HG23	7:B:406:PC1:C15	2.00	0.91
5:I:138:THR:H	6:I:408:UND:H111	1.36	0.90
7:J:104:PC1:C26	7:J:104:PC1:C33	2.45	0.90
2:E:16:MET:HA	2:E:19:LYS:HE2	1.53	0.90
5:B:140:GLN:HG2	5:B:146:ALA:HB2	1.56	0.88
1:F:37:ASP:OD2	1:F:40:ASP:HB2	1.74	0.87
3:G:40:ALA:HB2	3:G:47:PRO:HD3	1.54	0.87
5:I:203:VAL:HG23	7:I:409:PC1:H151	1.56	0.86
5:I:205:LEU:HG	5:I:208:PRO:HG3	1.56	0.86
3:J:10:GLN:HA	3:J:13:GLN:NE2	1.91	0.86
2:E:16:MET:HA	2:E:19:LYS:CE	2.06	0.85
5:I:203:VAL:HG23	7:I:409:PC1:C15	2.07	0.84
5:I:140:GLN:HG2	5:I:146:ALA:HB2	1.60	0.83
3:G:25:TRP:CD2	7:G:104:PC1:C15	2.59	0.82
1:F:30:GLY:HA2	1:F:33:ARG:NH1	1.94	0.82
7:G:104:PC1:H351	7:G:104:PC1:C28	2.10	0.81
3:J:25:TRP:CD2	7:J:104:PC1:C15	2.58	0.81
3:G:6:LYS:O	3:G:9:LYS:HG2	1.80	0.81
7:J:104:PC1:H351	7:J:104:PC1:C28	2.10	0.81
1:A:66:ASP:O	1:A:67:LEU:HD23	1.83	0.79
5:B:203:VAL:CG2	7:B:406:PC1:H151	2.14	0.78
7:G:104:PC1:H241	7:G:104:PC1:H322	1.66	0.78
7:J:104:PC1:H241	7:J:104:PC1:H322	1.66	0.77
3:J:7:GLU:HA	3:J:10:GLN:HE22	1.49	0.77
1:A:30:GLY:HA2	1:A:33:ARG:NH2	2.00	0.77
5:I:142:SER:HB2	5:I:143:PRO:HD2	1.67	0.76
3:G:25:TRP:NE1	7:G:104:PC1:H153	2.01	0.76
3:G:16:PHE:O	3:G:20:GLN:HG3	1.85	0.76
7:G:104:PC1:H262	7:G:104:PC1:C33	2.13	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:138:THR:N	6:B:405:UND:H111	1.99	0.76
2:E:15:GLU:OE2	2:E:18:ARG:HB2	1.86	0.76
3:J:12:LEU:O	3:J:15:LEU:N	2.20	0.75
3:J:40:ALA:HB2	3:J:47:PRO:HD3	1.67	0.75
5:I:82:THR:OG1	5:I:85:GLU:HG3	1.87	0.75
3:G:25:TRP:CD1	7:G:104:PC1:H153	2.23	0.74
3:J:25:TRP:NE1	7:J:104:PC1:H153	2.02	0.74
3:J:10:GLN:HA	3:J:13:GLN:HE22	1.53	0.73
3:J:16:PHE:O	3:J:20:GLN:HG3	1.87	0.73
3:J:25:TRP:CD1	7:J:104:PC1:H153	2.25	0.72
7:J:104:PC1:H262	7:J:104:PC1:C33	2.13	0.72
1:A:30:GLY:O	1:A:33:ARG:HG2	1.90	0.71
5:I:203:VAL:CG2	7:I:409:PC1:H151	2.20	0.71
5:B:142:SER:HB2	5:B:143:PRO:HD2	1.71	0.71
3:G:5:SER:O	3:G:8:ALA:N	2.20	0.71
2:D:13:PRO:HB2	2:D:15:GLU:OE1	1.91	0.70
3:J:53:LEU:HD21	7:B:401:PC1:H3C1	1.72	0.70
3:G:25:TRP:CE2	7:G:104:PC1:H153	2.27	0.69
4:H:102:GLU:HG3	5:I:312:LEU:HD22	1.75	0.69
4:C:101:PHE:HZ	5:I:360:ILE:HD11	1.58	0.69
3:J:53:LEU:HD21	7:B:401:PC1:C3C	2.23	0.69
7:B:408:PC1:H341	7:B:408:PC1:H252	1.75	0.69
5:I:91:LYS:NZ	5:I:287:GLU:OE1	2.25	0.68
7:I:406:PC1:H341	7:I:406:PC1:H252	1.75	0.68
4:H:68:ASP:OD1	4:H:69:LEU:N	2.27	0.67
4:C:72:PHE:CZ	7:C:202:PC1:H151	2.29	0.67
3:G:6:LYS:HB2	3:G:9:LYS:NZ	2.07	0.67
4:C:63:ALA:HA	4:C:66:THR:HG22	1.76	0.67
5:I:138:THR:N	6:I:408:UND:H111	2.06	0.67
3:G:12:LEU:HD23	5:I:211:LEU:HD11	1.77	0.66
2:E:16:MET:SD	2:E:20:MET:HE2	2.35	0.66
7:J:105:PC1:H132	5:B:184:LYS:CG	2.24	0.66
3:J:25:TRP:CE2	7:J:104:PC1:H153	2.27	0.66
5:I:141:LEU:HD12	5:I:167:GLN:HE22	1.60	0.66
4:C:72:PHE:CZ	7:C:202:PC1:C15	2.79	0.65
4:C:113:GLN:O	4:C:116:GLN:HG3	1.95	0.65
3:J:5:SER:HB3	3:J:8:ALA:HB3	1.79	0.65
3:J:10:GLN:HA	3:J:13:GLN:CD	2.21	0.65
2:E:22:GLU:O	2:E:25:ILE:HG22	1.96	0.65
3:G:41:ASP:HB2	3:G:44:MET:HE2	1.79	0.64
5:B:203:VAL:CG2	7:B:406:PC1:C15	2.74	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:91:LYS:NZ	5:B:287:GLU:OE1	2.30	0.64
5:I:88:ARG:O	5:I:92:GLU:HG2	1.97	0.64
3:J:25:TRP:CE3	7:J:104:PC1:H151	2.32	0.63
7:B:408:PC1:H341	7:B:408:PC1:H282	1.82	0.62
3:G:51:SER:HB3	5:I:109:LEU:HD22	1.81	0.62
4:H:72:PHE:CZ	7:H:202:PC1:C15	2.82	0.62
5:B:358:LEU:HD22	7:I:410:PC1:H282	1.80	0.62
4:C:98:PRO:HG3	7:I:410:PC1:H392	1.82	0.61
3:G:25:TRP:CE3	7:G:104:PC1:H151	2.35	0.61
3:G:40:ALA:HB2	3:G:47:PRO:CD	2.28	0.61
3:J:7:GLU:HA	3:J:10:GLN:NE2	2.15	0.61
5:I:249:SER:O	5:I:250:LEU:HD23	2.00	0.61
7:I:406:PC1:H341	7:I:406:PC1:H282	1.82	0.61
3:G:44:MET:HB3	3:G:45:PRO:HD2	1.82	0.60
4:H:72:PHE:CZ	7:H:202:PC1:H151	2.35	0.60
3:J:5:SER:HB3	3:J:8:ALA:CB	2.30	0.60
2:D:31:PHE:HB2	5:I:248:MET:HE2	1.84	0.60
1:F:54:ALA:HB1	7:B:402:PC1:H2D1	1.82	0.60
5:I:203:VAL:CG2	7:I:409:PC1:C15	2.80	0.60
3:J:41:ASP:HB2	3:J:44:MET:HE2	1.83	0.60
2:E:31:PHE:HB2	5:B:248:MET:HE2	1.83	0.59
3:J:51:SER:HB3	5:B:109:LEU:HD22	1.84	0.59
2:E:16:MET:HA	2:E:19:LYS:NZ	2.17	0.59
7:H:203:PC1:O14	5:B:156:ASN:HB2	2.02	0.59
1:A:54:ALA:HB1	7:A:102:PC1:H2D1	1.84	0.59
4:H:101:PHE:HZ	5:B:360:ILE:HD11	1.67	0.59
3:J:20:GLN:HE21	7:J:105:PC1:H31	1.67	0.59
2:E:22:GLU:HA	2:E:25:ILE:HG22	1.85	0.59
3:G:7:GLU:HA	3:G:10:GLN:NE2	2.18	0.58
1:F:40:ASP:OD2	1:F:42:ARG:HB2	2.02	0.58
5:B:256:LEU:HG	5:B:257:ASN:H	1.68	0.58
5:B:214:SER:HA	5:B:239:ARG:O	2.04	0.57
5:B:236:VAL:O	5:B:246:THR:HA	2.03	0.57
1:A:28:LEU:O	1:A:31:VAL:HG22	2.03	0.57
1:F:59:ALA:HB1	5:B:284:VAL:HG21	1.86	0.57
2:E:18:ARG:HH21	2:E:22:GLU:HG2	1.69	0.57
3:G:12:LEU:HD23	5:I:211:LEU:CD1	2.34	0.57
2:E:15:GLU:O	2:E:19:LYS:NZ	2.31	0.57
5:I:124:ILE:HG13	5:I:125:GLY:N	2.21	0.56
5:B:124:ILE:HG13	5:B:125:GLY:N	2.19	0.56
5:I:141:LEU:HD12	5:I:167:GLN:NE2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:51:SER:HB3	5:I:109:LEU:CD2	2.36	0.56
5:I:137:GLY:CA	6:I:408:UND:H111	2.36	0.56
3:G:4:LEU:HD11	3:G:9:LYS:HB3	1.87	0.56
4:H:86:TRP:HB2	7:H:203:PC1:H11	1.88	0.56
3:J:13:GLN:O	3:J:17:LYS:HG2	2.06	0.56
7:J:105:PC1:H132	5:B:184:LYS:HG2	1.88	0.55
4:C:113:GLN:O	4:C:117:ARG:HG3	2.06	0.55
5:B:157:SER:HA	7:B:401:PC1:H141	1.88	0.55
4:H:105:LYS:HG2	4:H:109:GLU:OE2	2.06	0.55
2:D:15:GLU:HG2	2:D:16:MET:N	2.20	0.55
5:I:236:VAL:O	5:I:246:THR:HA	2.06	0.55
7:I:406:PC1:H341	7:I:406:PC1:C28	2.37	0.55
7:B:408:PC1:H341	7:B:408:PC1:C28	2.37	0.55
3:J:51:SER:HB3	5:B:109:LEU:CD2	2.37	0.54
5:B:137:GLY:CA	6:B:405:UND:H111	2.36	0.54
5:B:249:SER:O	5:B:250:LEU:HD23	2.08	0.54
1:F:51:LEU:HD11	7:B:402:PC1:H32	1.89	0.54
4:H:86:TRP:HB2	7:H:203:PC1:C1	2.37	0.54
3:G:25:TRP:NE1	7:G:104:PC1:C15	2.62	0.54
4:C:96:VAL:O	4:C:99:VAL:HG12	2.07	0.54
5:B:181:GLN:O	5:B:182:GLN:C	2.48	0.54
5:B:167:GLN:OE1	5:B:173:ARG:NH2	2.41	0.54
2:D:14:GLU:OE2	2:D:18:ARG:HB2	2.08	0.53
7:G:104:PC1:H281	7:G:104:PC1:C35	2.32	0.53
1:A:37:ASP:OD1	1:A:40:ASP:N	2.41	0.53
3:J:38:ARG:NH1	3:J:38:ARG:HG2	2.24	0.53
5:B:137:GLY:HA2	6:B:405:UND:C11	2.39	0.53
1:A:26:ASP:OD1	1:A:27:TRP:N	2.42	0.53
5:I:223:GLN:HG2	5:I:224:SER:N	2.24	0.53
4:C:105:LYS:HG2	4:C:109:GLU:OE2	2.08	0.53
5:B:348:ARG:NH2	7:B:402:PC1:O14	2.41	0.53
1:A:59:ALA:HB1	5:I:284:VAL:HG21	1.89	0.53
3:J:40:ALA:HB2	3:J:46:GLU:HA	1.91	0.53
1:F:30:GLY:O	1:F:33:ARG:HG2	2.08	0.52
4:C:78:TYR:CZ	4:C:82:ARG:HD2	2.43	0.52
5:I:137:GLY:HA2	6:I:408:UND:C11	2.39	0.52
5:I:256:LEU:HD12	5:I:259:TRP:HZ2	1.74	0.52
5:B:226:THR:HB	5:B:227:PRO:CD	2.40	0.52
3:G:7:GLU:HG2	3:G:8:ALA:N	2.23	0.52
1:A:45:LEU:CD2	5:I:297:THR:HG21	2.39	0.52
2:D:24:VAL:HG22	5:I:246:THR:HG23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:77:LEU:HD13	5:I:224:SER:O	2.10	0.52
4:C:72:PHE:CE1	7:C:202:PC1:H151	2.44	0.52
2:D:19:LYS:HD2	2:D:22:GLU:OE2	2.10	0.52
3:J:38:ARG:HG2	3:J:38:ARG:HH11	1.75	0.52
3:J:40:ALA:HB2	3:J:47:PRO:CD	2.37	0.52
1:A:51:LEU:HD11	7:A:102:PC1:H32	1.92	0.51
5:I:95:PRO:HD2	5:I:317:SER:HB3	1.92	0.51
5:I:226:THR:HB	5:I:227:PRO:CD	2.40	0.51
4:C:101:PHE:HZ	5:I:360:ILE:CD1	2.23	0.51
4:H:72:PHE:CE1	7:H:202:PC1:H151	2.45	0.51
5:I:256:LEU:HD12	5:I:259:TRP:CZ2	2.45	0.51
1:A:45:LEU:HD23	5:I:297:THR:HG21	1.93	0.51
4:H:101:PHE:HZ	5:B:360:ILE:CD1	2.24	0.51
5:B:304:GLN:HG3	5:B:315:LYS:HG2	1.93	0.51
3:J:5:SER:OG	3:J:7:GLU:HG3	2.11	0.51
5:B:223:GLN:HG2	5:B:224:SER:N	2.24	0.51
5:I:341:LEU:HD23	5:I:356:PHE:HB3	1.93	0.51
2:D:21:ARG:NH2	5:I:244:GLU:OE1	2.44	0.50
2:E:34:TYR:OH	5:B:232:GLY:O	2.20	0.50
3:J:53:LEU:HD21	7:B:401:PC1:H3C2	1.93	0.50
2:E:19:LYS:O	2:E:22:GLU:HG3	2.11	0.50
5:I:220:HIS:CE1	5:I:234:GLU:HG3	2.46	0.50
1:F:56:VAL:O	1:F:60:ARG:HG3	2.12	0.50
5:B:341:LEU:HD23	5:B:356:PHE:HB3	1.93	0.50
5:I:141:LEU:HD12	5:I:167:GLN:OE1	2.11	0.50
5:I:304:GLN:HG3	5:I:315:LYS:HG2	1.93	0.50
3:G:20:GLN:HE21	7:G:105:PC1:H31	1.77	0.49
3:G:41:ASP:CB	3:G:44:MET:HE2	2.43	0.49
3:G:53:LEU:HD21	7:I:402:PC1:H3C2	1.95	0.49
3:J:44:MET:HB3	3:J:45:PRO:HD2	1.95	0.49
5:B:95:PRO:HD2	5:B:317:SER:HB3	1.94	0.49
7:G:103:PC1:H361	7:G:103:PC1:H332	1.63	0.48
2:D:21:ARG:HA	2:D:21:ARG:HE	1.78	0.48
5:B:348:ARG:HH12	7:B:402:PC1:H111	1.77	0.48
3:G:4:LEU:HD12	3:G:4:LEU:O	2.14	0.48
5:I:328:LEU:HB3	7:I:410:PC1:H2I1	1.96	0.48
5:I:207:ASN:N	5:I:208:PRO:HD3	2.28	0.48
3:G:25:TRP:CG	7:G:104:PC1:C15	2.97	0.48
3:G:25:TRP:CZ2	7:G:104:PC1:C15	2.94	0.48
3:J:25:TRP:CG	7:J:104:PC1:C15	2.97	0.48
5:I:258:ASN:OD1	5:I:258:ASN:C	2.54	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:16:PHE:HE2	5:I:211:LEU:HD13	1.79	0.47
5:I:160:LEU:HG	5:I:161:ASN:N	2.29	0.47
7:B:401:PC1:O22	7:B:401:PC1:O11	2.32	0.47
1:F:57:TRP:CZ3	7:B:402:PC1:H2G2	2.49	0.47
1:A:59:ALA:HB1	5:I:284:VAL:CG2	2.45	0.47
5:B:137:GLY:CA	6:B:405:UND:C11	2.93	0.47
5:I:101:VAL:HA	5:I:356:PHE:O	2.15	0.47
6:I:405:UND:H113	7:I:409:PC1:H232	1.97	0.47
1:A:27:TRP:O	1:A:30:GLY:N	2.48	0.46
1:A:37:ASP:O	1:A:43:ARG:HD2	2.15	0.46
4:C:102:GLU:HG3	5:B:312:LEU:HD22	1.97	0.46
7:I:406:PC1:H252	7:I:406:PC1:C34	2.45	0.46
2:D:21:ARG:HH21	5:I:244:GLU:CD	2.24	0.46
4:H:78:TYR:CZ	4:H:82:ARG:HD2	2.51	0.46
7:B:406:PC1:H232	6:B:407:UND:H113	1.98	0.46
5:B:270:MET:HG2	5:B:271:HIS:N	2.31	0.46
4:C:69:LEU:HD13	7:C:202:PC1:O12	2.16	0.46
7:J:105:PC1:C13	5:B:184:LYS:CG	2.92	0.46
5:B:101:VAL:HA	5:B:356:PHE:O	2.15	0.46
5:I:270:MET:HG2	5:I:271:HIS:N	2.30	0.46
4:C:101:PHE:CZ	5:I:360:ILE:HD11	2.44	0.45
5:I:156:ASN:ND2	7:I:403:PC1:H111	2.31	0.45
7:I:410:PC1:H152	7:I:410:PC1:O13	2.16	0.45
3:G:25:TRP:CD1	7:G:104:PC1:C15	2.97	0.45
5:I:137:GLY:CA	6:I:408:UND:C11	2.94	0.45
7:G:103:PC1:H3G1	7:G:103:PC1:H3D1	1.67	0.45
5:I:212:VAL:HG12	5:I:212:VAL:O	2.15	0.45
2:E:21:ARG:NH2	5:B:244:GLU:OE1	2.49	0.45
4:C:71:LEU:C	4:C:71:LEU:HD23	2.41	0.45
4:H:71:LEU:C	4:H:71:LEU:HD23	2.42	0.45
2:D:40:VAL:HG22	2:D:40:VAL:O	2.17	0.45
1:F:59:ALA:HB1	5:B:284:VAL:CG2	2.46	0.45
2:E:21:ARG:HH21	5:B:244:GLU:CD	2.25	0.45
3:G:7:GLU:OE1	3:G:7:GLU:N	2.45	0.45
4:H:106:LEU:C	4:H:106:LEU:HD23	2.42	0.45
1:A:36:THR:HG22	1:A:36:THR:O	2.17	0.44
5:B:164:VAL:O	5:B:175:LYS:HA	2.17	0.44
5:B:137:GLY:HA2	6:B:405:UND:H113	2.00	0.44
5:B:109:LEU:HD12	5:B:113:PHE:CE2	2.53	0.44
5:B:226:THR:HB	5:B:227:PRO:HD2	2.00	0.44
5:B:240:ARG:HB3	5:B:241:PRO:CD	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:296:ASP:OD1	5:I:296:ASP:C	2.60	0.44
4:C:63:ALA:HA	4:C:66:THR:CG2	2.46	0.44
3:J:25:TRP:CD1	7:J:104:PC1:C15	2.98	0.44
3:J:9:LYS:O	3:J:13:GLN:OE1	2.34	0.44
7:G:103:PC1:H152	7:G:103:PC1:H111	1.68	0.44
7:J:104:PC1:H351	7:J:104:PC1:H282	1.99	0.44
7:B:408:PC1:H252	7:B:408:PC1:C34	2.45	0.44
5:I:147:PHE:HB3	5:I:148:PRO:HA	2.00	0.44
2:D:13:PRO:HD2	2:D:15:GLU:OE2	2.18	0.44
4:C:106:LEU:C	4:C:106:LEU:HD23	2.43	0.44
3:J:41:ASP:HB2	3:J:44:MET:CE	2.48	0.43
7:G:103:PC1:H382	7:G:103:PC1:H352	1.79	0.43
4:H:114:LEU:C	4:H:114:LEU:HD23	2.43	0.43
7:G:104:PC1:H133	7:I:402:PC1:H222	2.00	0.43
4:H:73:VAL:HG23	4:H:74:ALA:N	2.34	0.43
5:I:141:LEU:HD12	5:I:167:GLN:CD	2.44	0.43
5:I:249:SER:C	5:I:250:LEU:HD23	2.43	0.43
4:C:114:LEU:C	4:C:114:LEU:HD23	2.44	0.43
5:B:332:LEU:HD22	7:I:410:PC1:H12	2.00	0.43
7:H:203:PC1:C15	5:B:126:GLU:OE2	2.67	0.43
3:J:25:TRP:CZ2	7:J:104:PC1:C15	2.94	0.43
2:D:19:LYS:O	2:D:22:GLU:HG3	2.17	0.43
7:J:103:PC1:H292	7:J:103:PC1:H262	1.85	0.43
1:F:26:ASP:OD1	1:F:27:TRP:N	2.52	0.43
5:I:164:VAL:O	5:I:175:LYS:HA	2.18	0.43
5:I:226:THR:HB	5:I:227:PRO:HD2	2.00	0.43
1:A:30:GLY:HA2	1:A:33:ARG:HH22	1.81	0.43
3:J:6:LYS:HD3	3:J:6:LYS:C	2.44	0.43
5:I:141:LEU:C	5:I:141:LEU:HD23	2.44	0.43
4:H:115:GLN:HA	4:H:118:GLN:HB3	2.01	0.42
2:E:37:LEU:HD23	2:E:37:LEU:HA	1.86	0.42
7:J:104:PC1:H281	7:J:104:PC1:C35	2.32	0.42
5:B:240:ARG:HB3	5:B:241:PRO:HD2	2.01	0.42
5:B:256:LEU:O	5:B:257:ASN:C	2.62	0.42
7:J:105:PC1:C13	5:B:184:LYS:HG3	2.49	0.42
5:I:137:GLY:HA2	6:I:408:UND:H113	2.02	0.42
5:I:177:ALA:O	5:I:178:ILE:HG12	2.20	0.42
3:J:52:LEU:HD23	5:B:115:VAL:HG21	2.00	0.42
7:B:402:PC1:H291	7:B:402:PC1:H251	2.02	0.42
2:D:21:ARG:O	2:D:25:ILE:HG12	2.20	0.42
7:J:103:PC1:H132	7:J:103:PC1:H111	1.69	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:307:LEU:HD12	5:B:312:LEU:HD23	2.01	0.42
5:I:307:LEU:HD12	5:I:312:LEU:HD23	2.02	0.42
7:I:403:PC1:O32	7:I:403:PC1:O21	2.38	0.42
1:A:66:ASP:C	1:A:67:LEU:HD23	2.44	0.42
7:A:102:PC1:H251	7:A:102:PC1:H291	2.02	0.42
3:J:10:GLN:HA	3:J:13:GLN:OE1	2.20	0.42
7:I:406:PC1:H341	7:I:406:PC1:C27	2.50	0.42
5:B:341:LEU:HD23	5:B:356:PHE:CB	2.49	0.41
7:B:408:PC1:H341	7:B:408:PC1:C27	2.50	0.41
2:E:40:VAL:O	2:E:40:VAL:HG22	2.19	0.41
4:C:70:SER:O	4:C:73:VAL:HG22	2.20	0.41
5:I:341:LEU:HD23	5:I:356:PHE:CB	2.50	0.41
3:G:5:SER:HB3	3:G:7:GLU:OE2	2.20	0.41
1:A:41:PHE:CE1	5:I:297:THR:HG23	2.55	0.41
4:C:73:VAL:HG23	4:C:74:ALA:N	2.35	0.41
4:C:99:VAL:HG21	5:B:305:LEU:HD13	2.01	0.41
4:C:99:VAL:O	4:C:103:THR:HG23	2.20	0.41
5:B:105:VAL:O	5:B:116:ASN:HA	2.20	0.41
5:B:215:GLY:O	5:B:216:ILE:HD13	2.20	0.41
1:F:57:TRP:HZ3	7:B:402:PC1:H2G2	1.85	0.41
4:H:72:PHE:CZ	7:H:202:PC1:H152	2.55	0.41
5:B:112:HIS:O	5:B:135:TYR:HA	2.21	0.41
5:B:220:HIS:CE1	5:B:234:GLU:HG3	2.55	0.41
5:I:240:ARG:NH2	5:I:243:GLU:HG3	2.36	0.41
5:I:156:ASN:HD22	7:I:403:PC1:H111	1.85	0.41
1:A:27:TRP:C	1:A:30:GLY:H	2.29	0.41
4:H:69:LEU:CD1	7:H:202:PC1:O12	2.56	0.41
4:C:112:GLN:OE1	4:C:113:GLN:N	2.54	0.41
3:J:41:ASP:CB	3:J:44:MET:HE2	2.50	0.41
7:J:103:PC1:H3G1	7:J:103:PC1:H3D1	1.73	0.41
5:B:141:LEU:HD23	5:B:141:LEU:C	2.46	0.41
5:B:155:ASP:OD1	5:B:155:ASP:C	2.64	0.41
5:B:182:GLN:H	5:B:182:GLN:CD	2.29	0.41
5:I:155:ASP:OD1	5:I:155:ASP:C	2.64	0.41
7:I:403:PC1:H153	7:I:403:PC1:O13	2.21	0.41
4:H:113:GLN:HA	4:H:116:GLN:OE1	2.21	0.41
3:G:52:LEU:HD23	5:I:115:VAL:HG21	2.02	0.40
4:C:82:ARG:NH2	7:I:403:PC1:H332	2.36	0.40
5:B:99:GLU:HA	5:B:354:CYS:O	2.22	0.40
5:I:257:ASN:O	5:I:258:ASN:OD1	2.39	0.40
1:F:65:ILE:HG13	1:F:66:ASP:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.82	0.40
2:D:22:GLU:OE2	2:D:23:ASP:OD1	2.40	0.40
3:J:25:TRP:CE2	7:J:104:PC1:H152	2.46	0.40
3:G:9:LYS:HG3	3:G:10:GLN:N	2.36	0.40
5:B:147:PHE:HB3	5:B:148:PRO:HA	2.04	0.40
5:B:249:SER:C	5:B:250:LEU:HD23	2.46	0.40
5:B:331:LYS:C	5:B:333:PRO:HD3	2.47	0.40
1:F:41:PHE:CE2	1:F:45:LEU:HD11	2.57	0.40
2:E:16:MET:CA	2:E:19:LYS:HE2	2.37	0.40
4:H:114:LEU:O	4:H:118:GLN:N	2.55	0.40
5:B:230:ALA:HB3	5:B:253:LYS:HG2	2.04	0.40
5:I:109:LEU:HD12	5:I:113:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	41/74 (55%)	40 (98%)	1 (2%)	0	100	100
1	F	41/74 (55%)	40 (98%)	1 (2%)	0	100	100
2	D	34/51 (67%)	34 (100%)	0	0	100	100
2	E	34/51 (67%)	34 (100%)	0	0	100	100
3	G	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
3	J	52/55 (94%)	48 (92%)	4 (8%)	0	100	100
4	C	55/142 (39%)	54 (98%)	1 (2%)	0	100	100
4	H	54/142 (38%)	52 (96%)	2 (4%)	0	100	100
5	B	284/361 (79%)	272 (96%)	12 (4%)	0	100	100
5	I	284/361 (79%)	277 (98%)	7 (2%)	0	100	100
All	All	931/1366 (68%)	901 (97%)	30 (3%)	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	35/59 (59%)	35 (100%)	0	100	100
1	F	35/59 (59%)	35 (100%)	0	100	100
2	D	35/48 (73%)	35 (100%)	0	100	100
2	E	35/48 (73%)	35 (100%)	0	100	100
3	G	45/46 (98%)	44 (98%)	1 (2%)	47	71
3	J	45/46 (98%)	45 (100%)	0	100	100
4	C	49/115 (43%)	48 (98%)	1 (2%)	50	74
4	H	49/115 (43%)	48 (98%)	1 (2%)	50	74
5	B	238/288 (83%)	237 (100%)	1 (0%)	89	96
5	I	238/288 (83%)	238 (100%)	0	100	100
All	All	804/1112 (72%)	800 (100%)	4 (0%)	85	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	46	GLU
4	H	76	LYS
4	C	76	LYS
5	B	86	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
3	G	13	GLN
4	H	111	GLN
3	J	20	GLN
5	B	112	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	257	ASN
5	I	106	ASN
5	I	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

43 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PC1	I	410	-	53,53,53	0.28	0	59,61,61	0.35	0
6	UND	F	103	-	10,10,10	0.11	0	9,9,9	0.07	0
7	PC1	G	103	-	53,53,53	0.26	0	59,61,61	0.28	0
6	UND	G	102	-	10,10,10	0.11	0	9,9,9	0.06	0
6	UND	I	407	-	10,10,10	0.11	0	9,9,9	0.06	0
6	UND	B	409	-	10,10,10	0.10	0	9,9,9	0.06	0
7	PC1	A	102	-	53,53,53	0.29	0	59,61,61	0.38	0
6	UND	B	407	-	10,10,10	0.13	0	9,9,9	0.08	0
7	PC1	J	103	-	53,53,53	0.27	0	59,61,61	0.29	0
7	PC1	B	401	-	53,53,53	0.28	0	59,61,61	0.36	0
7	PC1	H	201	-	53,53,53	0.26	0	59,61,61	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PC1	B	402	-	53,53,53	0.29	0	59,61,61	0.38	0
6	UND	F	101	-	10,10,10	0.12	0	9,9,9	0.06	0
7	PC1	C	201	-	53,53,53	0.26	0	59,61,61	0.42	0
7	PC1	B	404	-	53,53,53	0.28	0	59,61,61	0.41	0
6	UND	I	404	-	10,10,10	0.11	0	9,9,9	0.08	0
6	UND	A	101	-	10,10,10	0.11	0	9,9,9	0.07	0
7	PC1	I	409	-	53,53,53	0.25	0	59,61,61	0.35	0
7	PC1	G	101	-	53,53,53	0.26	0	59,61,61	0.32	0
6	UND	H	204	-	10,10,10	0.10	0	9,9,9	0.06	0
7	PC1	B	408	-	53,53,53	0.27	0	59,61,61	0.40	0
7	PC1	I	402	-	53,53,53	0.28	0	59,61,61	0.28	0
7	PC1	A	104	-	53,53,53	0.27	0	59,61,61	0.33	0
6	UND	I	408	-	10,10,10	0.10	0	9,9,9	0.07	0
7	PC1	F	102	-	53,53,53	0.27	0	59,61,61	0.33	0
7	PC1	G	104	-	53,53,53	0.26	0	59,61,61	0.37	0
6	UND	A	103	-	10,10,10	0.11	0	9,9,9	0.07	0
7	PC1	I	401	-	53,53,53	0.29	0	59,61,61	0.41	0
7	PC1	H	202	-	53,53,53	0.25	0	59,61,61	0.51	1 (1%)
7	PC1	B	406	-	53,53,53	0.26	0	59,61,61	0.35	0
7	PC1	I	406	-	53,53,53	0.27	0	59,61,61	0.40	0
7	PC1	H	203	-	53,53,53	0.30	0	59,61,61	0.34	0
7	PC1	I	403	-	53,53,53	0.30	0	59,61,61	0.33	0
6	UND	C	203	-	10,10,10	0.10	0	9,9,9	0.06	0
6	UND	B	403	-	10,10,10	0.12	0	9,9,9	0.09	0
7	PC1	J	104	-	53,53,53	0.27	0	59,61,61	0.37	0
6	UND	I	405	-	10,10,10	0.13	0	9,9,9	0.08	0
6	UND	B	405	-	10,10,10	0.10	0	9,9,9	0.07	0
7	PC1	G	105	-	53,53,53	0.29	0	59,61,61	0.31	0
7	PC1	J	101	-	53,53,53	0.26	0	59,61,61	0.31	0
7	PC1	J	105	-	53,53,53	0.29	0	59,61,61	0.31	0
6	UND	J	102	-	10,10,10	0.11	0	9,9,9	0.06	0
7	PC1	C	202	-	53,53,53	0.25	0	59,61,61	0.51	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PC1	I	410	-	-	14/57/57/57	-
6	UND	F	103	-	-	1/8/8/8	-
7	PC1	G	103	-	-	35/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UND	G	102	-	-	2/8/8/8	-
6	UND	I	407	-	-	2/8/8/8	-
6	UND	B	409	-	-	2/8/8/8	-
7	PC1	A	102	-	-	9/57/57/57	-
6	UND	B	407	-	-	0/8/8/8	-
7	PC1	J	103	-	-	33/57/57/57	-
7	PC1	B	401	-	-	14/57/57/57	-
7	PC1	H	201	-	-	18/57/57/57	-
7	PC1	B	402	-	-	9/57/57/57	-
6	UND	F	101	-	-	1/8/8/8	-
7	PC1	C	201	-	-	18/57/57/57	-
7	PC1	B	404	-	-	11/57/57/57	-
6	UND	I	404	-	-	0/8/8/8	-
6	UND	A	101	-	-	1/8/8/8	-
7	PC1	I	409	-	-	24/57/57/57	-
7	PC1	G	101	-	-	13/57/57/57	-
6	UND	H	204	-	-	0/8/8/8	-
7	PC1	B	408	-	-	19/57/57/57	-
7	PC1	I	402	-	-	17/57/57/57	-
7	PC1	A	104	-	-	29/57/57/57	-
6	UND	I	408	-	-	3/8/8/8	-
7	PC1	F	102	-	-	29/57/57/57	-
7	PC1	G	104	-	-	20/57/57/57	-
6	UND	A	103	-	-	1/8/8/8	-
7	PC1	I	401	-	-	11/57/57/57	-
7	PC1	H	202	-	-	18/57/57/57	-
7	PC1	B	406	-	-	24/57/57/57	-
7	PC1	I	406	-	-	19/57/57/57	-
7	PC1	H	203	-	-	16/57/57/57	-
7	PC1	I	403	-	-	8/57/57/57	-
6	UND	C	203	-	-	0/8/8/8	-
6	UND	B	403	-	-	1/8/8/8	-
7	PC1	J	104	-	-	20/57/57/57	-
6	UND	I	405	-	-	0/8/8/8	-
6	UND	B	405	-	-	3/8/8/8	-
7	PC1	G	105	-	-	7/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PC1	J	101	-	-	13/57/57/57	-
7	PC1	J	105	-	-	7/57/57/57	-
6	UND	J	102	-	-	2/8/8/8	-
7	PC1	C	202	-	-	18/57/57/57	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	202	PC1	O21-C2-C1	2.41	117.13	108.40
7	H	202	PC1	O21-C2-C1	2.41	117.13	108.40

There are no chirality outliers.

All (492) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	102	PC1	C22-C21-O21-C2
7	A	104	PC1	C11-O13-P-O12
7	A	104	PC1	C11-O13-P-O14
7	A	104	PC1	C11-O13-P-O11
7	A	104	PC1	O11-C1-C2-O21
7	A	104	PC1	C22-C21-O21-C2
7	F	102	PC1	C11-O13-P-O12
7	F	102	PC1	C11-O13-P-O14
7	F	102	PC1	C11-O13-P-O11
7	F	102	PC1	O11-C1-C2-O21
7	F	102	PC1	C22-C21-O21-C2
7	G	103	PC1	C11-O13-P-O12
7	G	103	PC1	C11-O13-P-O14
7	G	103	PC1	O13-C11-C12-N
7	G	104	PC1	C1-O11-P-O14
7	G	104	PC1	O13-C11-C12-N
7	G	104	PC1	O22-C21-O21-C2
7	G	104	PC1	C22-C21-O21-C2
7	G	105	PC1	O22-C21-O21-C2
7	G	105	PC1	C22-C21-O21-C2
7	H	201	PC1	C11-O13-P-O14
7	H	201	PC1	C11-O13-P-O11
7	H	201	PC1	O13-C11-C12-N
7	H	201	PC1	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	H	202	PC1	O13-C11-C12-N
7	H	202	PC1	O22-C21-O21-C2
7	C	201	PC1	C11-O13-P-O14
7	C	201	PC1	C11-O13-P-O11
7	C	201	PC1	O13-C11-C12-N
7	C	201	PC1	C22-C21-O21-C2
7	C	202	PC1	O13-C11-C12-N
7	C	202	PC1	O22-C21-O21-C2
7	J	103	PC1	C11-O13-P-O12
7	J	103	PC1	O13-C11-C12-N
7	J	104	PC1	C1-O11-P-O14
7	J	104	PC1	O13-C11-C12-N
7	J	104	PC1	O22-C21-O21-C2
7	J	104	PC1	C22-C21-O21-C2
7	J	105	PC1	O22-C21-O21-C2
7	J	105	PC1	C22-C21-O21-C2
7	B	402	PC1	C22-C21-O21-C2
7	B	404	PC1	O13-C11-C12-N
7	B	406	PC1	C11-O13-P-O14
7	B	406	PC1	C11-O13-P-O11
7	B	406	PC1	C1-O11-P-O14
7	B	406	PC1	O13-C11-C12-N
7	B	406	PC1	C22-C21-O21-C2
7	B	408	PC1	O13-C11-C12-N
7	B	408	PC1	C22-C21-O21-C2
7	I	401	PC1	O13-C11-C12-N
7	I	403	PC1	C11-O13-P-O14
7	I	406	PC1	O13-C11-C12-N
7	I	406	PC1	C22-C21-O21-C2
7	I	409	PC1	C11-O13-P-O14
7	I	409	PC1	C11-O13-P-O11
7	I	409	PC1	C1-O11-P-O14
7	I	409	PC1	O13-C11-C12-N
7	I	409	PC1	C22-C21-O21-C2
7	I	410	PC1	O32-C31-O31-C3
7	I	410	PC1	C32-C31-O31-C3
7	G	101	PC1	O32-C31-O31-C3
7	H	202	PC1	O32-C31-O31-C3
7	C	202	PC1	O32-C31-O31-C3
7	J	101	PC1	O32-C31-O31-C3
7	A	102	PC1	O22-C21-O21-C2
7	A	104	PC1	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	F	102	PC1	O22-C21-O21-C2
7	G	101	PC1	O22-C21-O21-C2
7	H	201	PC1	O22-C21-O21-C2
7	C	201	PC1	O22-C21-O21-C2
7	J	101	PC1	O22-C21-O21-C2
7	B	402	PC1	O22-C21-O21-C2
7	B	406	PC1	O22-C21-O21-C2
7	B	408	PC1	O22-C21-O21-C2
7	I	406	PC1	O22-C21-O21-C2
7	I	409	PC1	O22-C21-O21-C2
7	A	104	PC1	O32-C31-O31-C3
7	F	102	PC1	O32-C31-O31-C3
7	G	103	PC1	C32-C31-O31-C3
7	G	104	PC1	C32-C31-O31-C3
7	H	202	PC1	C32-C31-O31-C3
7	C	202	PC1	C32-C31-O31-C3
7	J	104	PC1	C32-C31-O31-C3
7	B	408	PC1	C32-C31-O31-C3
7	I	406	PC1	C32-C31-O31-C3
7	G	101	PC1	C22-C21-O21-C2
7	H	202	PC1	C22-C21-O21-C2
7	C	202	PC1	C22-C21-O21-C2
7	J	101	PC1	C22-C21-O21-C2
7	G	101	PC1	C32-C31-O31-C3
7	J	101	PC1	C32-C31-O31-C3
7	G	104	PC1	O32-C31-O31-C3
7	J	104	PC1	O32-C31-O31-C3
7	B	408	PC1	O32-C31-O31-C3
7	I	406	PC1	O32-C31-O31-C3
7	A	104	PC1	C32-C31-O31-C3
7	F	102	PC1	C32-C31-O31-C3
7	H	203	PC1	C32-C31-O31-C3
7	G	103	PC1	O32-C31-O31-C3
7	G	103	PC1	C26-C27-C28-C29
7	G	103	PC1	C35-C36-C37-C38
7	G	103	PC1	C28-C29-C2A-C2B
7	J	103	PC1	C26-C27-C28-C29
7	G	104	PC1	C2-C1-O11-P
7	J	104	PC1	C2-C1-O11-P
7	G	103	PC1	C3D-C3E-C3F-C3G
7	J	103	PC1	C28-C29-C2A-C2B
7	J	103	PC1	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	H	201	PC1	C32-C31-O31-C3
7	C	201	PC1	C32-C31-O31-C3
7	B	406	PC1	C32-C31-O31-C3
7	I	409	PC1	C32-C31-O31-C3
7	H	203	PC1	O32-C31-O31-C3
7	G	103	PC1	C31-C32-C33-C34
7	H	201	PC1	O32-C31-O31-C3
7	C	201	PC1	O32-C31-O31-C3
7	B	406	PC1	O32-C31-O31-C3
7	I	409	PC1	O32-C31-O31-C3
7	G	103	PC1	C33-C34-C35-C36
7	J	103	PC1	C32-C31-O31-C3
7	G	104	PC1	C21-C22-C23-C24
7	J	104	PC1	C21-C22-C23-C24
7	J	103	PC1	C35-C36-C37-C38
7	G	103	PC1	C11-C12-N-C15
7	I	410	PC1	C21-C22-C23-C24
7	I	402	PC1	C22-C21-O21-C2
7	G	101	PC1	C21-C22-C23-C24
7	J	101	PC1	C21-C22-C23-C24
7	J	103	PC1	O32-C31-O31-C3
7	I	403	PC1	C22-C21-O21-C2
7	G	103	PC1	C11-O13-P-O11
7	G	103	PC1	C1-O11-P-O13
7	G	104	PC1	C1-O11-P-O13
7	H	203	PC1	C11-O13-P-O11
7	J	103	PC1	C11-O13-P-O11
7	J	103	PC1	C1-O11-P-O13
7	J	104	PC1	C1-O11-P-O13
7	G	103	PC1	C3B-C3C-C3D-C3E
7	J	103	PC1	C31-C32-C33-C34
7	B	401	PC1	C22-C21-O21-C2
7	G	103	PC1	C39-C3A-C3B-C3C
7	G	104	PC1	C23-C24-C25-C26
7	H	202	PC1	C25-C26-C27-C28
7	H	202	PC1	C3E-C3F-C3G-C3H
7	H	203	PC1	C36-C37-C38-C39
7	C	202	PC1	C25-C26-C27-C28
7	C	202	PC1	C3E-C3F-C3G-C3H
7	J	104	PC1	C23-C24-C25-C26
7	B	406	PC1	C22-C23-C24-C25
7	B	406	PC1	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	408	PC1	C24-C25-C26-C27
7	I	406	PC1	C24-C25-C26-C27
7	I	409	PC1	C22-C23-C24-C25
7	I	409	PC1	C3B-C3C-C3D-C3E
7	J	103	PC1	C39-C3A-C3B-C3C
7	B	401	PC1	C29-C2A-C2B-C2C
7	H	202	PC1	C1-C2-O21-C21
7	C	202	PC1	C1-C2-O21-C21
7	I	402	PC1	O22-C21-O21-C2
7	I	403	PC1	O22-C21-O21-C2
7	H	202	PC1	C21-C22-C23-C24
7	C	202	PC1	C21-C22-C23-C24
7	J	103	PC1	C2A-C2B-C2C-C2D
7	J	103	PC1	C2C-C2D-C2E-C2F
7	B	401	PC1	C24-C25-C26-C27
7	I	402	PC1	C21-C22-C23-C24
7	B	404	PC1	C3A-C3B-C3C-C3D
7	I	401	PC1	C3A-C3B-C3C-C3D
7	A	104	PC1	C29-C2A-C2B-C2C
7	F	102	PC1	C29-C2A-C2B-C2C
7	B	408	PC1	C32-C33-C34-C35
7	I	402	PC1	C2A-C2B-C2C-C2D
7	I	406	PC1	C32-C33-C34-C35
7	I	410	PC1	C33-C34-C35-C36
7	G	101	PC1	C26-C27-C28-C29
7	J	101	PC1	C26-C27-C28-C29
7	F	102	PC1	C32-C33-C34-C35
7	H	201	PC1	C33-C34-C35-C36
7	C	201	PC1	C33-C34-C35-C36
7	G	103	PC1	C11-C12-N-C14
7	A	104	PC1	C32-C33-C34-C35
7	G	101	PC1	C33-C34-C35-C36
7	J	101	PC1	C33-C34-C35-C36
7	B	401	PC1	C32-C33-C34-C35
7	B	404	PC1	C37-C38-C39-C3A
7	I	401	PC1	C37-C38-C39-C3A
7	I	410	PC1	C3A-C3B-C3C-C3D
6	B	403	UND	C2-C3-C4-C5
7	A	102	PC1	C2A-C2B-C2C-C2D
7	B	402	PC1	C2A-C2B-C2C-C2D
7	B	408	PC1	C27-C28-C29-C2A
7	I	406	PC1	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	104	PC1	C2E-C2F-C2G-C2H
7	F	102	PC1	C2E-C2F-C2G-C2H
7	J	103	PC1	C3E-C3F-C3G-C3H
7	B	406	PC1	C24-C25-C26-C27
7	I	409	PC1	C24-C25-C26-C27
7	B	406	PC1	C37-C38-C39-C3A
7	I	409	PC1	C37-C38-C39-C3A
7	I	410	PC1	C29-C2A-C2B-C2C
7	G	103	PC1	C3E-C3F-C3G-C3H
7	G	101	PC1	C28-C29-C2A-C2B
7	J	101	PC1	C28-C29-C2A-C2B
7	G	103	PC1	C24-C25-C26-C27
7	B	401	PC1	O22-C21-O21-C2
7	G	103	PC1	C2C-C2D-C2E-C2F
6	A	101	UND	C3-C4-C5-C6
6	F	101	UND	C3-C4-C5-C6
7	A	104	PC1	C3C-C3D-C3E-C3F
7	F	102	PC1	C3C-C3D-C3E-C3F
7	A	104	PC1	C3E-C3F-C3G-C3H
7	F	102	PC1	C3E-C3F-C3G-C3H
7	H	201	PC1	C39-C3A-C3B-C3C
7	C	201	PC1	C39-C3A-C3B-C3C
7	B	401	PC1	C31-C32-C33-C34
7	B	401	PC1	C3D-C3E-C3F-C3G
7	H	201	PC1	C3B-C3C-C3D-C3E
7	C	201	PC1	C3B-C3C-C3D-C3E
7	B	406	PC1	C34-C35-C36-C37
7	I	409	PC1	C34-C35-C36-C37
7	G	103	PC1	C2A-C2B-C2C-C2D
7	B	404	PC1	C3E-C3F-C3G-C3H
7	I	401	PC1	C3E-C3F-C3G-C3H
7	G	103	PC1	C11-C12-N-C13
7	J	103	PC1	C11-C12-N-C13
7	H	203	PC1	C26-C27-C28-C29
7	B	406	PC1	C39-C3A-C3B-C3C
7	I	409	PC1	C39-C3A-C3B-C3C
7	I	409	PC1	C36-C37-C38-C39
7	H	203	PC1	C22-C21-O21-C2
7	H	203	PC1	C35-C36-C37-C38
7	J	103	PC1	C22-C23-C24-C25
7	B	406	PC1	C36-C37-C38-C39
7	H	203	PC1	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	103	PC1	C2-C1-O11-P
7	A	104	PC1	O11-C1-C2-C3
7	F	102	PC1	O11-C1-C2-C3
7	G	104	PC1	O11-C1-C2-C3
7	J	104	PC1	O11-C1-C2-C3
6	B	405	UND	C6-C7-C8-C9
6	I	408	UND	C6-C7-C8-C9
7	J	103	PC1	C24-C25-C26-C27
7	I	401	PC1	C2E-C2F-C2G-C2H
7	B	404	PC1	C2E-C2F-C2G-C2H
7	J	103	PC1	C33-C34-C35-C36
7	A	104	PC1	C24-C25-C26-C27
7	F	102	PC1	C24-C25-C26-C27
7	B	408	PC1	C3F-C3G-C3H-C3I
7	I	406	PC1	C3F-C3G-C3H-C3I
7	G	103	PC1	C2-C1-O11-P
7	B	406	PC1	C31-C32-C33-C34
7	I	409	PC1	C31-C32-C33-C34
7	A	104	PC1	C38-C39-C3A-C3B
7	F	102	PC1	C38-C39-C3A-C3B
7	G	103	PC1	C22-C23-C24-C25
7	I	406	PC1	C3B-C3C-C3D-C3E
7	B	408	PC1	C3B-C3C-C3D-C3E
7	G	103	PC1	O11-C1-C2-C3
7	J	103	PC1	O11-C1-C2-C3
6	B	409	UND	C2-C3-C4-C5
7	H	201	PC1	C36-C37-C38-C39
7	C	201	PC1	C36-C37-C38-C39
7	I	403	PC1	C32-C31-O31-C3
6	I	407	UND	C2-C3-C4-C5
7	G	105	PC1	C2E-C2F-C2G-C2H
7	J	105	PC1	C2E-C2F-C2G-C2H
7	B	408	PC1	C38-C39-C3A-C3B
7	I	406	PC1	C38-C39-C3A-C3B
6	B	405	UND	C7-C8-C9-C10
6	I	408	UND	C7-C8-C9-C10
7	H	202	PC1	C2E-C2F-C2G-C2H
7	C	202	PC1	C2E-C2F-C2G-C2H
7	H	202	PC1	C1-C2-C3-O31
7	C	202	PC1	C1-C2-C3-O31
7	G	104	PC1	C31-C32-C33-C34
7	J	104	PC1	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	103	PC1	C2B-C2C-C2D-C2E
7	B	408	PC1	C28-C29-C2A-C2B
7	I	406	PC1	C28-C29-C2A-C2B
7	I	410	PC1	C2E-C2F-C2G-C2H
6	F	103	UND	C6-C7-C8-C9
7	I	406	PC1	C21-C22-C23-C24
6	A	103	UND	C6-C7-C8-C9
7	H	202	PC1	C2A-C2B-C2C-C2D
7	C	202	PC1	C2A-C2B-C2C-C2D
7	A	102	PC1	C22-C23-C24-C25
7	B	402	PC1	C22-C23-C24-C25
7	G	104	PC1	O11-C1-C2-O21
7	G	105	PC1	O11-C1-C2-O21
7	J	104	PC1	O11-C1-C2-O21
7	J	105	PC1	O11-C1-C2-O21
7	B	408	PC1	C21-C22-C23-C24
7	G	103	PC1	C2B-C2C-C2D-C2E
7	H	202	PC1	O21-C2-C3-O31
7	C	202	PC1	O21-C2-C3-O31
7	F	102	PC1	C26-C27-C28-C29
7	A	104	PC1	C26-C27-C28-C29
7	H	202	PC1	C23-C24-C25-C26
7	C	202	PC1	C23-C24-C25-C26
6	I	407	UND	C6-C7-C8-C9
6	B	409	UND	C6-C7-C8-C9
7	A	104	PC1	C2-C1-O11-P
7	F	102	PC1	C2-C1-O11-P
7	I	410	PC1	C2-C1-O11-P
7	I	409	PC1	C32-C33-C34-C35
7	B	406	PC1	C32-C33-C34-C35
7	B	408	PC1	C3A-C3B-C3C-C3D
7	I	406	PC1	C3A-C3B-C3C-C3D
7	H	201	PC1	C3C-C3D-C3E-C3F
7	C	201	PC1	C3C-C3D-C3E-C3F
7	A	102	PC1	C26-C27-C28-C29
7	B	402	PC1	C26-C27-C28-C29
7	I	406	PC1	C2B-C2C-C2D-C2E
7	G	103	PC1	C3A-C3B-C3C-C3D
7	B	408	PC1	C2B-C2C-C2D-C2E
7	J	103	PC1	C11-C12-N-C14
7	J	103	PC1	C3A-C3B-C3C-C3D
7	B	408	PC1	C3-C2-O21-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	I	406	PC1	C3-C2-O21-C21
6	G	102	UND	C7-C8-C9-C10
6	J	102	UND	C7-C8-C9-C10
7	B	406	PC1	C1-C2-C3-O31
7	I	409	PC1	C1-C2-C3-O31
7	H	201	PC1	O11-C1-C2-O21
7	C	201	PC1	O11-C1-C2-O21
7	H	201	PC1	C24-C25-C26-C27
7	C	201	PC1	C24-C25-C26-C27
7	B	408	PC1	C3C-C3D-C3E-C3F
7	I	406	PC1	C3C-C3D-C3E-C3F
6	G	102	UND	C11-C10-C9-C8
6	J	102	UND	C11-C10-C9-C8
7	H	201	PC1	C38-C39-C3A-C3B
7	C	201	PC1	C38-C39-C3A-C3B
7	J	104	PC1	C2F-C2G-C2H-C2I
7	G	104	PC1	C2F-C2G-C2H-C2I
7	B	401	PC1	C3B-C3C-C3D-C3E
7	I	410	PC1	C3B-C3C-C3D-C3E
7	F	102	PC1	C3B-C3C-C3D-C3E
7	A	104	PC1	C3B-C3C-C3D-C3E
7	B	404	PC1	C11-O13-P-O11
7	B	406	PC1	C1-O11-P-O13
7	I	401	PC1	C11-O13-P-O11
7	I	409	PC1	C1-O11-P-O13
7	G	101	PC1	C2-C1-O11-P
7	H	202	PC1	C2-C1-O11-P
7	C	202	PC1	C2-C1-O11-P
7	J	101	PC1	C2-C1-O11-P
7	G	103	PC1	C1-O11-P-O14
7	G	104	PC1	C1-O11-P-O12
7	H	203	PC1	C11-O13-P-O14
7	J	103	PC1	C1-O11-P-O14
7	J	104	PC1	C1-O11-P-O12
7	J	103	PC1	C3B-C3C-C3D-C3E
7	G	105	PC1	O11-C1-C2-C3
7	J	105	PC1	O11-C1-C2-C3
7	A	104	PC1	C12-C11-O13-P
7	F	102	PC1	C12-C11-O13-P
7	B	406	PC1	C12-C11-O13-P
7	I	402	PC1	C12-C11-O13-P
7	I	409	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	I	410	PC1	C12-C11-O13-P
7	A	104	PC1	C22-C23-C24-C25
7	G	103	PC1	C32-C33-C34-C35
7	F	102	PC1	C22-C23-C24-C25
7	G	103	PC1	O11-C1-C2-O21
7	J	103	PC1	O11-C1-C2-O21
7	I	402	PC1	O11-C1-C2-O21
7	A	104	PC1	C21-C22-C23-C24
7	F	102	PC1	C21-C22-C23-C24
7	G	101	PC1	O13-C11-C12-N
7	J	101	PC1	O13-C11-C12-N
7	I	402	PC1	O13-C11-C12-N
7	B	406	PC1	O21-C2-C3-O31
7	I	409	PC1	O21-C2-C3-O31
7	I	402	PC1	C3F-C3G-C3H-C3I
7	I	410	PC1	C27-C28-C29-C2A
7	F	102	PC1	C35-C36-C37-C38
7	A	104	PC1	C35-C36-C37-C38
7	B	406	PC1	C33-C34-C35-C36
7	I	409	PC1	C33-C34-C35-C36
7	H	202	PC1	C27-C28-C29-C2A
7	C	202	PC1	C27-C28-C29-C2A
7	I	403	PC1	O32-C31-O31-C3
7	H	203	PC1	O22-C21-O21-C2
7	G	101	PC1	C23-C24-C25-C26
7	B	401	PC1	C3F-C3G-C3H-C3I
7	J	101	PC1	C23-C24-C25-C26
7	J	103	PC1	C36-C37-C38-C39
7	H	201	PC1	C3-C2-O21-C21
7	C	201	PC1	C3-C2-O21-C21
7	I	402	PC1	C2-C1-O11-P
7	J	103	PC1	C11-C12-N-C15
7	A	102	PC1	C28-C29-C2A-C2B
7	H	203	PC1	C28-C29-C2A-C2B
7	B	402	PC1	C28-C29-C2A-C2B
7	A	102	PC1	C1-O11-P-O13
7	B	402	PC1	C1-O11-P-O13
7	I	402	PC1	C11-O13-P-O11
7	I	410	PC1	C1-O11-P-O13
7	J	103	PC1	C2D-C2E-C2F-C2G
7	I	403	PC1	C27-C28-C29-C2A
7	F	102	PC1	C2D-C2E-C2F-C2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	104	PC1	C2D-C2E-C2F-C2G
7	G	103	PC1	O22-C21-O21-C2
7	A	104	PC1	C23-C24-C25-C26
7	F	102	PC1	C23-C24-C25-C26
7	A	102	PC1	O21-C2-C3-O31
7	B	402	PC1	O21-C2-C3-O31
7	G	105	PC1	C23-C24-C25-C26
7	J	105	PC1	C23-C24-C25-C26
7	J	104	PC1	C34-C35-C36-C37
7	G	104	PC1	C34-C35-C36-C37
6	I	408	UND	C4-C5-C6-C7
6	B	405	UND	C4-C5-C6-C7
7	B	401	PC1	C1-C2-O21-C21
7	I	402	PC1	C1-C2-O21-C21
7	I	402	PC1	C3-C2-O21-C21
7	H	202	PC1	C3C-C3D-C3E-C3F
7	C	202	PC1	C3C-C3D-C3E-C3F
7	A	104	PC1	O21-C2-C3-O31
7	F	102	PC1	O21-C2-C3-O31
7	J	103	PC1	C38-C39-C3A-C3B
7	I	403	PC1	C31-C32-C33-C34
7	G	103	PC1	C22-C21-O21-C2
7	H	203	PC1	C3F-C3G-C3H-C3I
7	H	201	PC1	C25-C26-C27-C28
7	C	201	PC1	C25-C26-C27-C28
7	B	408	PC1	O31-C31-C32-C33
7	I	406	PC1	O31-C31-C32-C33
7	I	402	PC1	C29-C2A-C2B-C2C
7	G	101	PC1	C2A-C2B-C2C-C2D
7	J	101	PC1	C2A-C2B-C2C-C2D
7	J	103	PC1	C32-C33-C34-C35
7	C	202	PC1	C32-C33-C34-C35
7	G	104	PC1	O31-C31-C32-C33
7	J	104	PC1	O31-C31-C32-C33
7	H	202	PC1	C32-C33-C34-C35
7	A	104	PC1	O21-C21-C22-C23
7	F	102	PC1	O21-C21-C22-C23
7	G	101	PC1	C2E-C2F-C2G-C2H
7	J	101	PC1	C2E-C2F-C2G-C2H
7	B	404	PC1	O21-C21-C22-C23
7	I	401	PC1	O21-C21-C22-C23
7	I	402	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	406	PC1	O21-C21-C22-C23
7	G	104	PC1	O21-C21-C22-C23
7	J	104	PC1	O21-C21-C22-C23
7	I	409	PC1	O21-C21-C22-C23
7	I	402	PC1	C2-C3-O31-C31
7	A	102	PC1	C2D-C2E-C2F-C2G
7	B	402	PC1	C2D-C2E-C2F-C2G
7	C	201	PC1	C22-C23-C24-C25
7	H	201	PC1	C22-C23-C24-C25
7	A	104	PC1	O22-C21-C22-C23
7	F	102	PC1	O22-C21-C22-C23
7	B	404	PC1	C32-C33-C34-C35
7	I	401	PC1	C32-C33-C34-C35
7	I	402	PC1	C2E-C2F-C2G-C2H
7	B	408	PC1	O32-C31-C32-C33
7	I	406	PC1	O32-C31-C32-C33
7	G	103	PC1	C2D-C2E-C2F-C2G
7	I	410	PC1	C1-O11-P-O14
7	G	104	PC1	O32-C31-C32-C33
7	J	104	PC1	O32-C31-C32-C33
7	H	203	PC1	O22-C21-C22-C23
7	G	103	PC1	C23-C24-C25-C26
7	B	404	PC1	O22-C21-C22-C23
7	B	406	PC1	O22-C21-C22-C23
7	I	401	PC1	O22-C21-C22-C23
7	I	409	PC1	O22-C21-C22-C23
7	I	410	PC1	O31-C31-C32-C33
7	G	103	PC1	C12-C11-O13-P
7	B	404	PC1	C12-C11-O13-P
7	I	401	PC1	C12-C11-O13-P
7	G	104	PC1	O22-C21-C22-C23
7	J	104	PC1	O22-C21-C22-C23
7	F	102	PC1	C33-C34-C35-C36
7	B	401	PC1	O21-C21-C22-C23
7	A	104	PC1	C33-C34-C35-C36
7	I	402	PC1	C2D-C2E-C2F-C2G
7	B	404	PC1	C25-C26-C27-C28
7	I	401	PC1	C25-C26-C27-C28
7	H	203	PC1	C21-C22-C23-C24
7	H	203	PC1	O21-C21-C22-C23
7	B	401	PC1	O31-C31-C32-C33
7	I	403	PC1	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	103	PC1	O22-C21-O21-C2
7	H	203	PC1	C3D-C3E-C3F-C3G
7	J	105	PC1	C38-C39-C3A-C3B
7	G	105	PC1	C38-C39-C3A-C3B
7	B	401	PC1	O22-C21-C22-C23
7	B	401	PC1	O32-C31-C32-C33

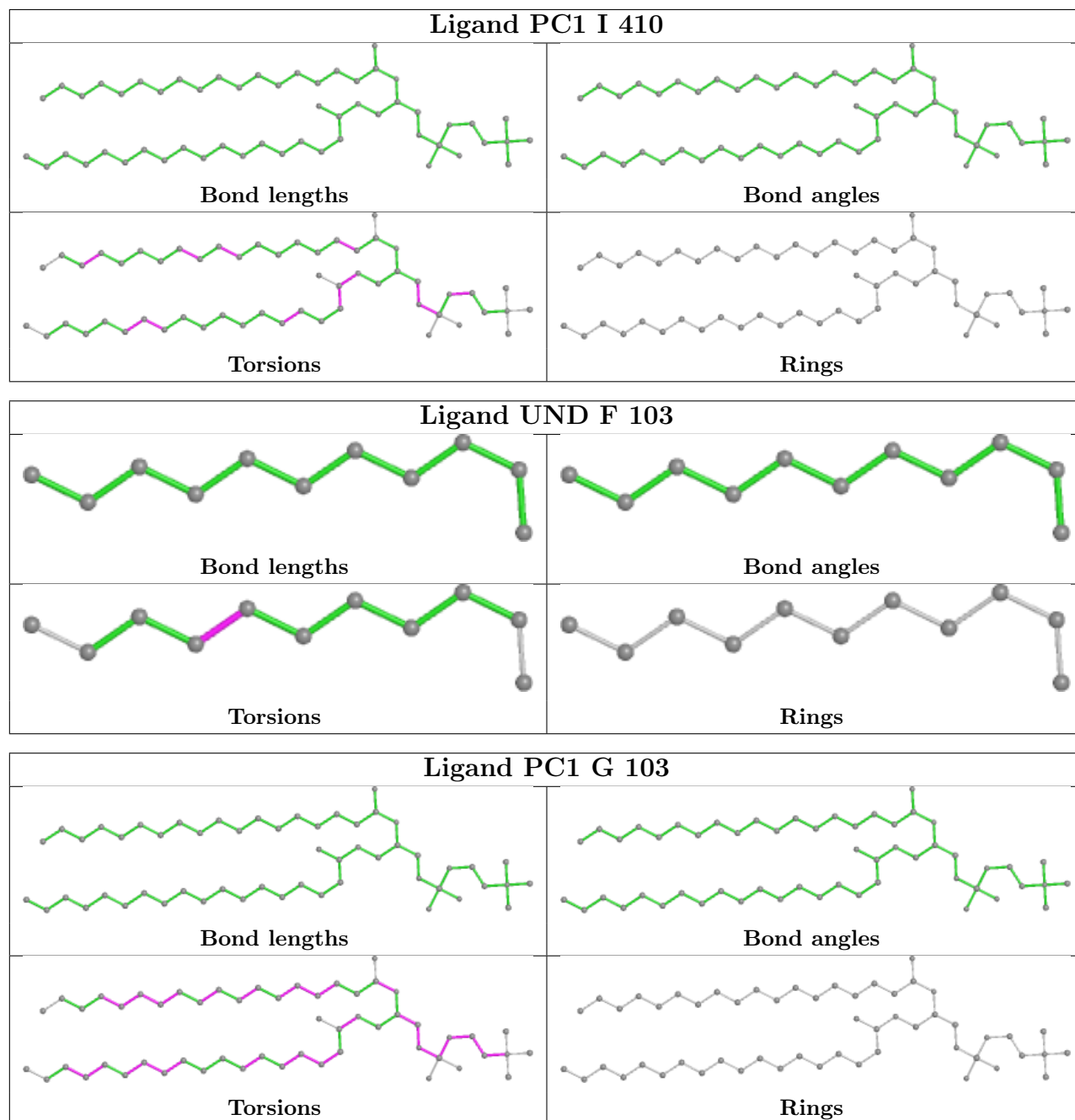
There are no ring outliers.

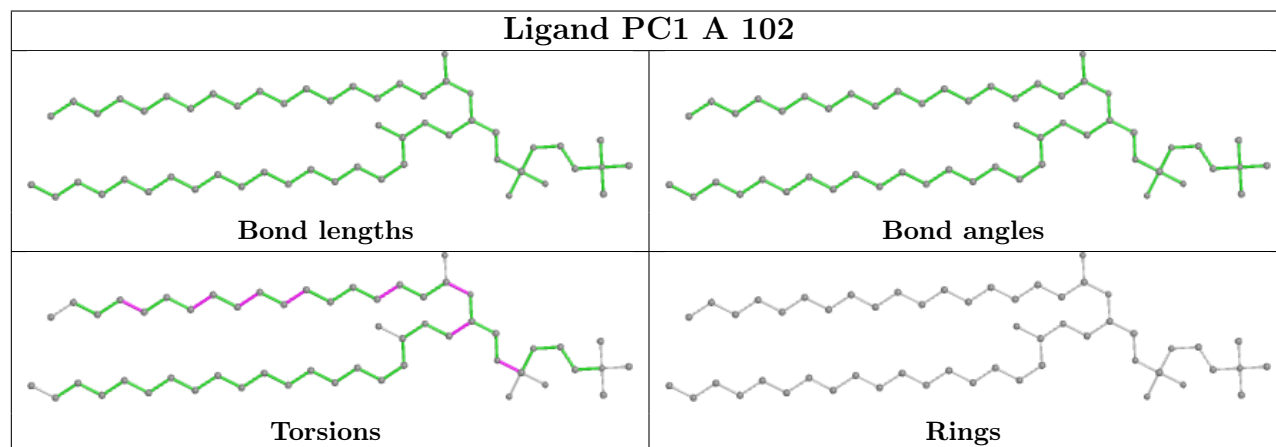
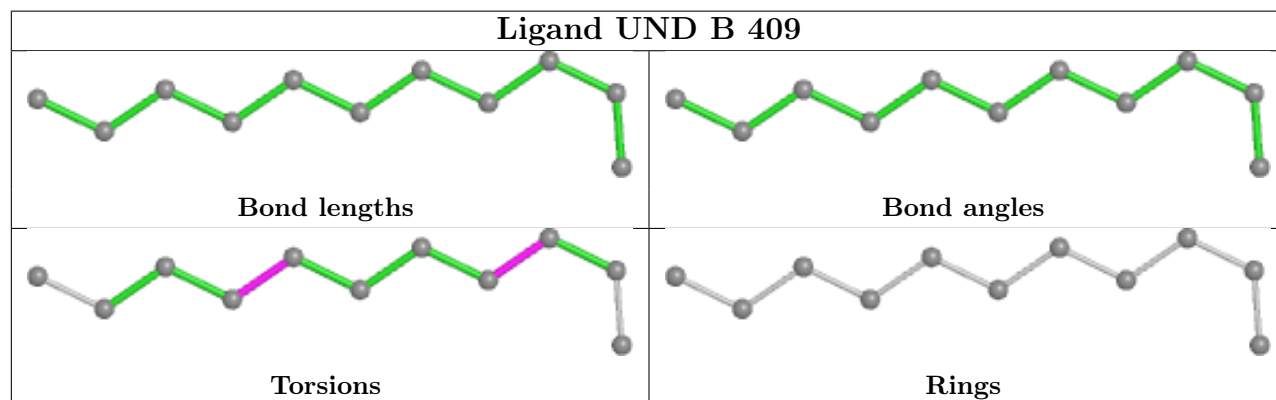
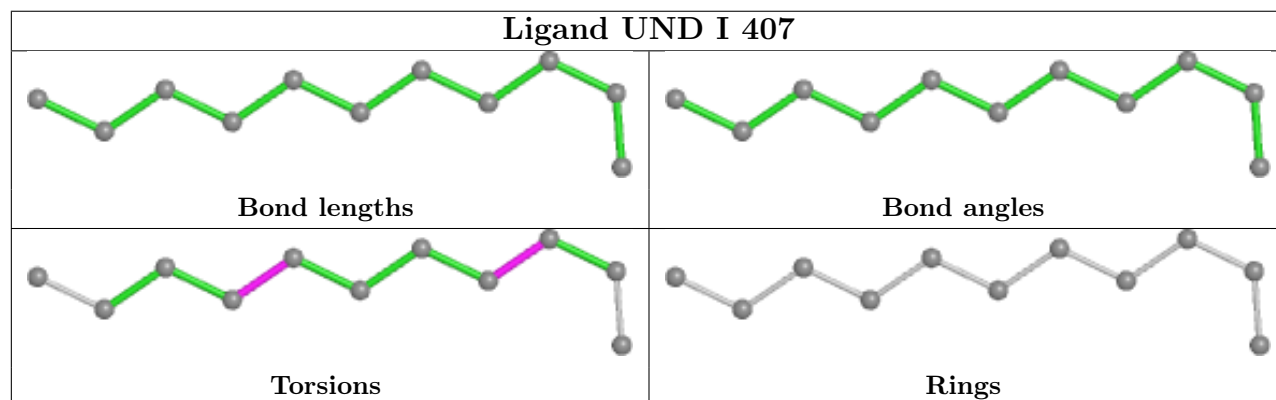
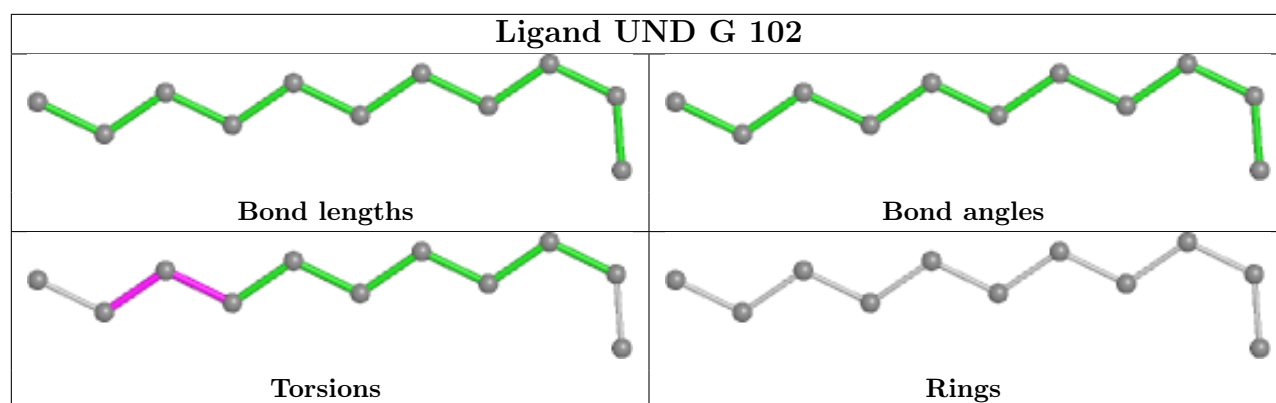
23 monomers are involved in 131 short contacts:

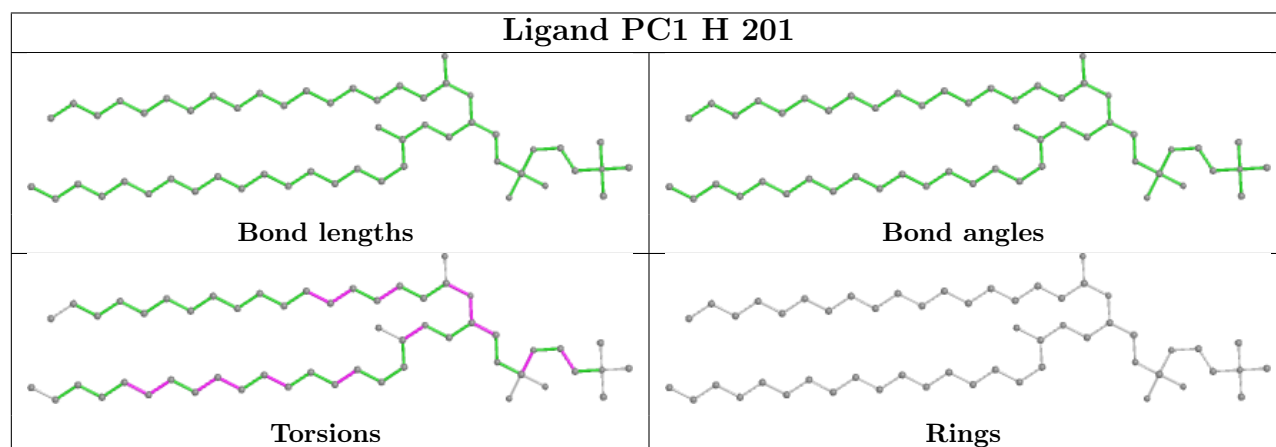
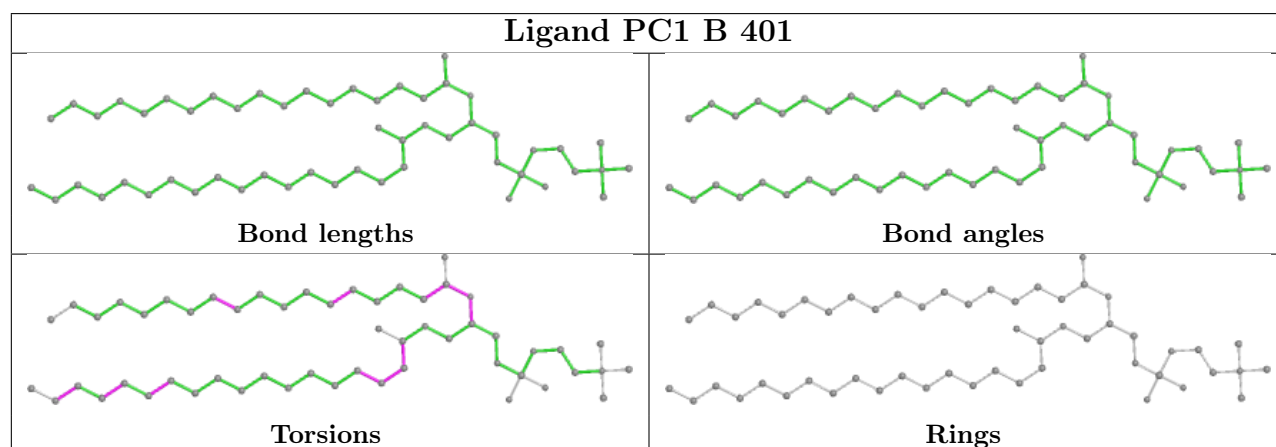
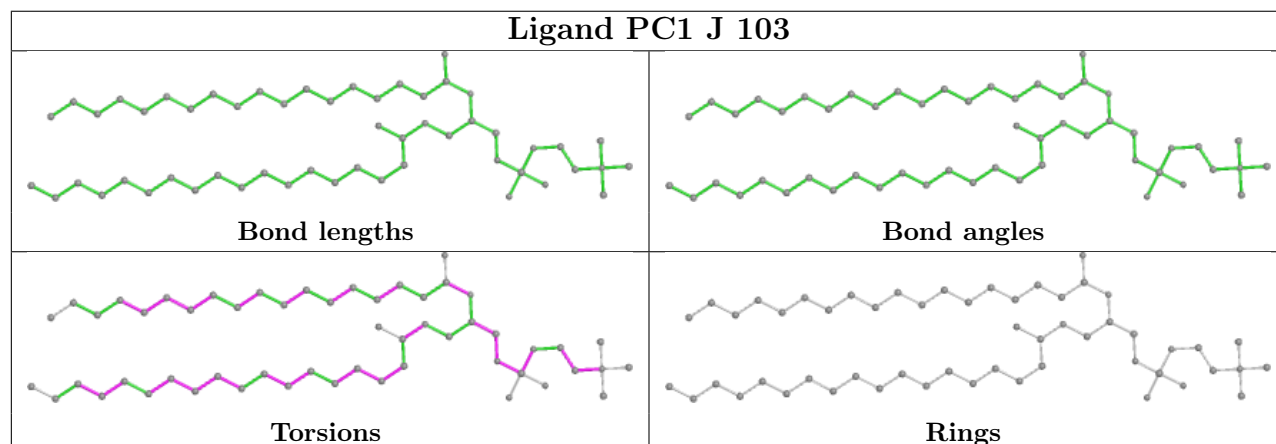
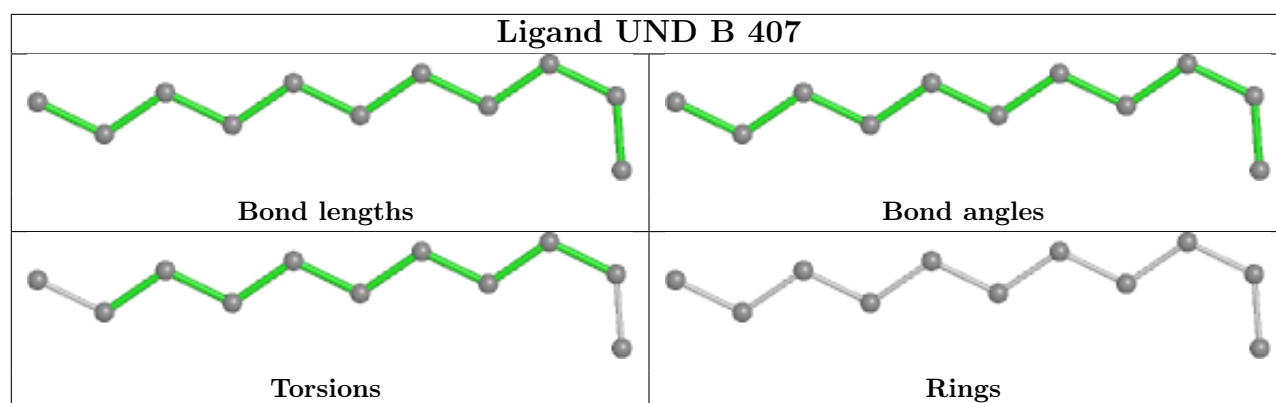
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	410	PC1	5	0
7	G	103	PC1	4	0
7	A	102	PC1	3	0
6	B	407	UND	1	0
7	J	103	PC1	3	0
7	B	401	PC1	5	0
7	B	402	PC1	7	0
7	I	409	PC1	5	0
7	B	408	PC1	5	0
7	I	402	PC1	2	0
6	I	408	UND	6	0
7	G	104	PC1	23	0
7	H	202	PC1	6	0
7	B	406	PC1	5	0
7	I	406	PC1	5	0
7	H	203	PC1	4	0
7	I	403	PC1	5	0
7	J	104	PC1	23	0
6	I	405	UND	1	0
6	B	405	UND	6	0
7	G	105	PC1	1	0
7	J	105	PC1	5	0
7	C	202	PC1	4	0

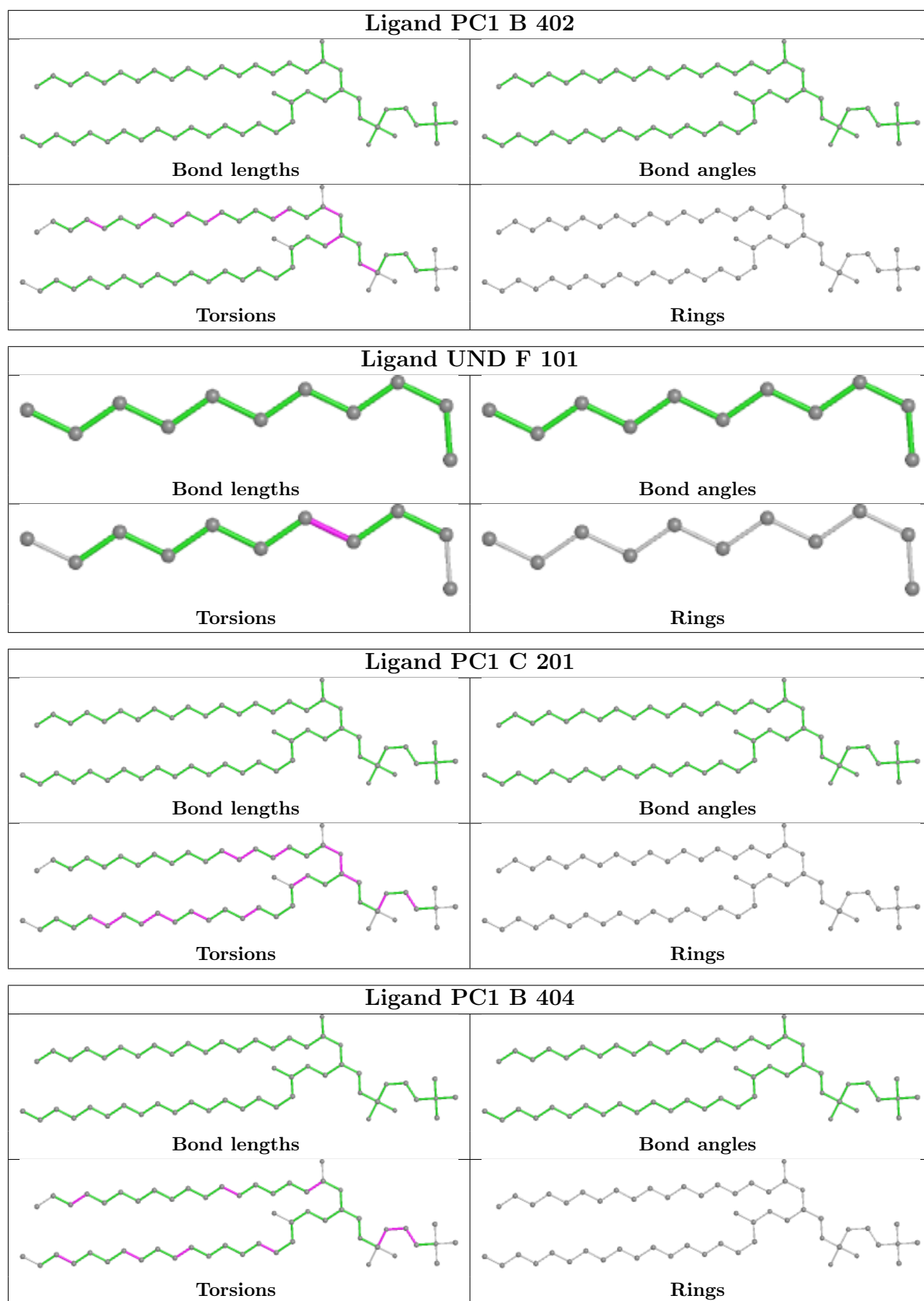
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

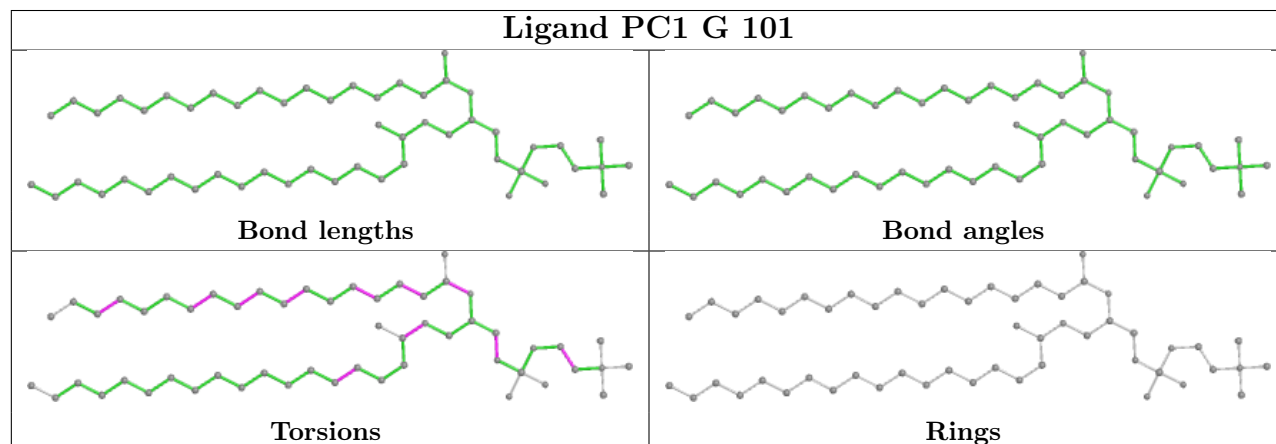
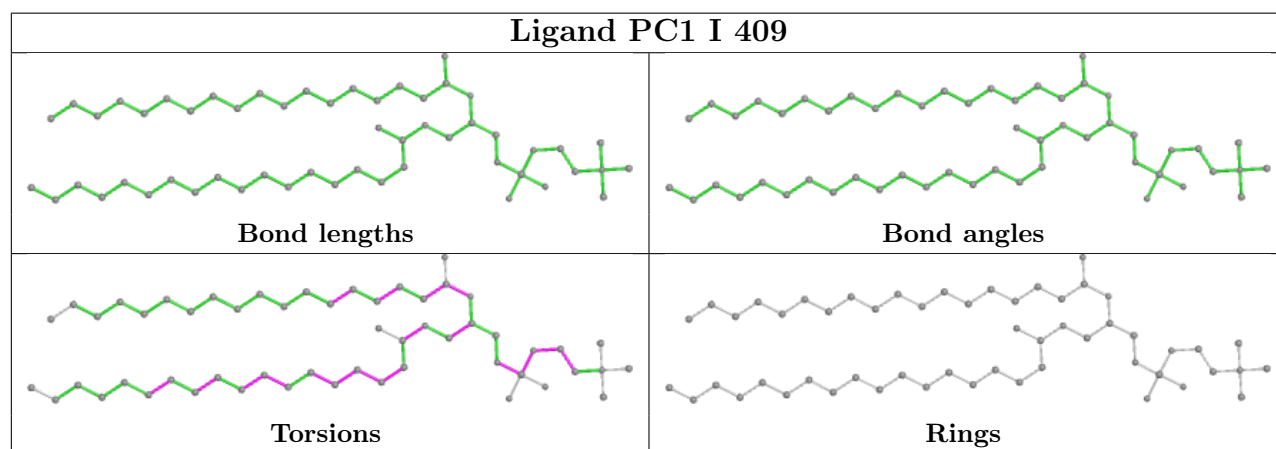
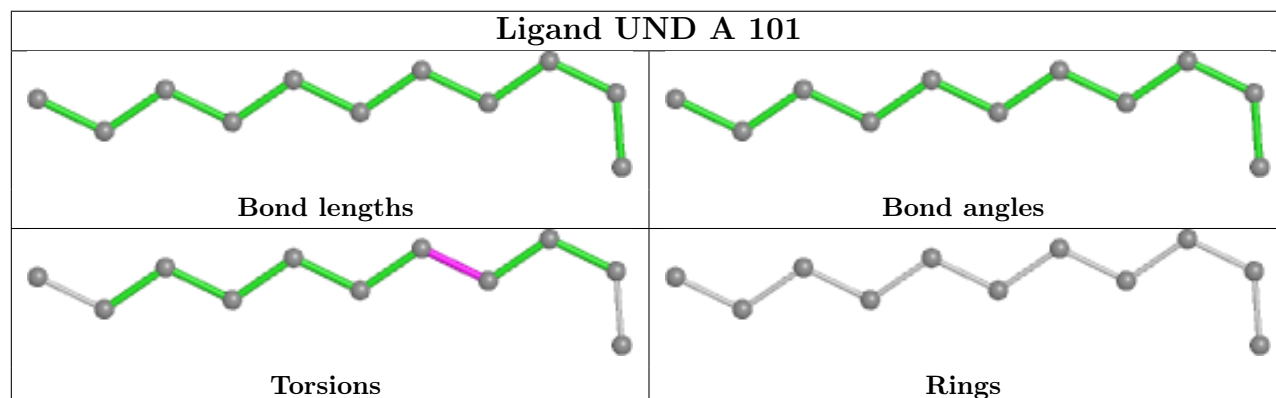
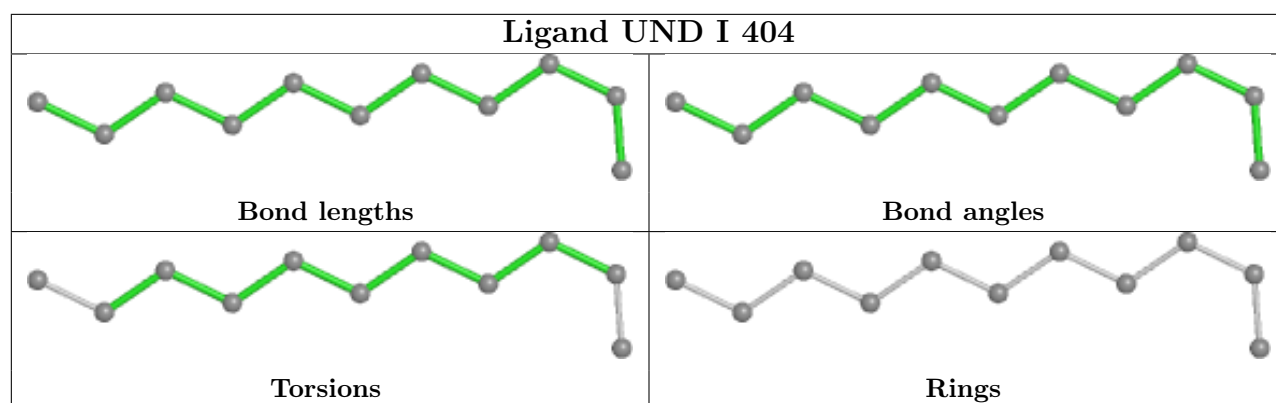
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

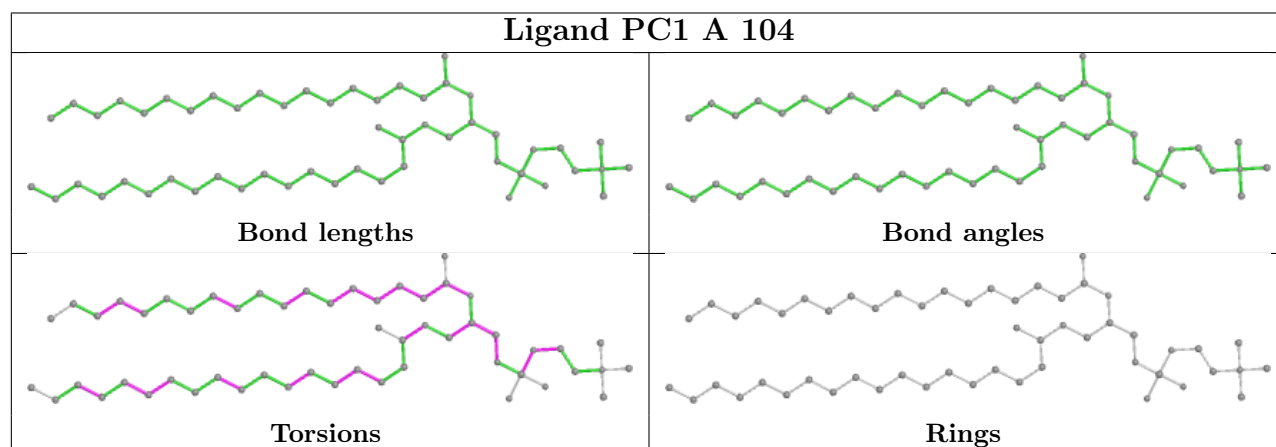
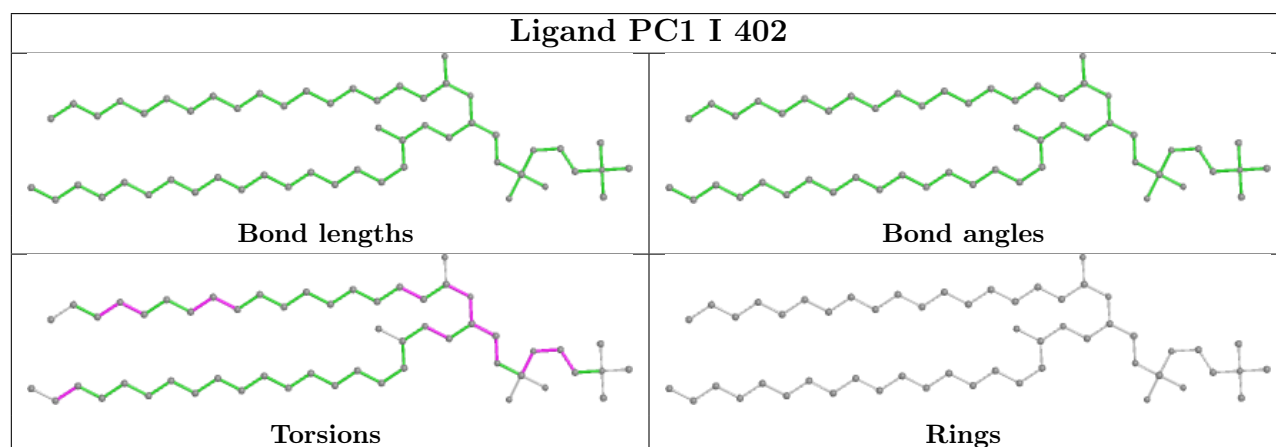
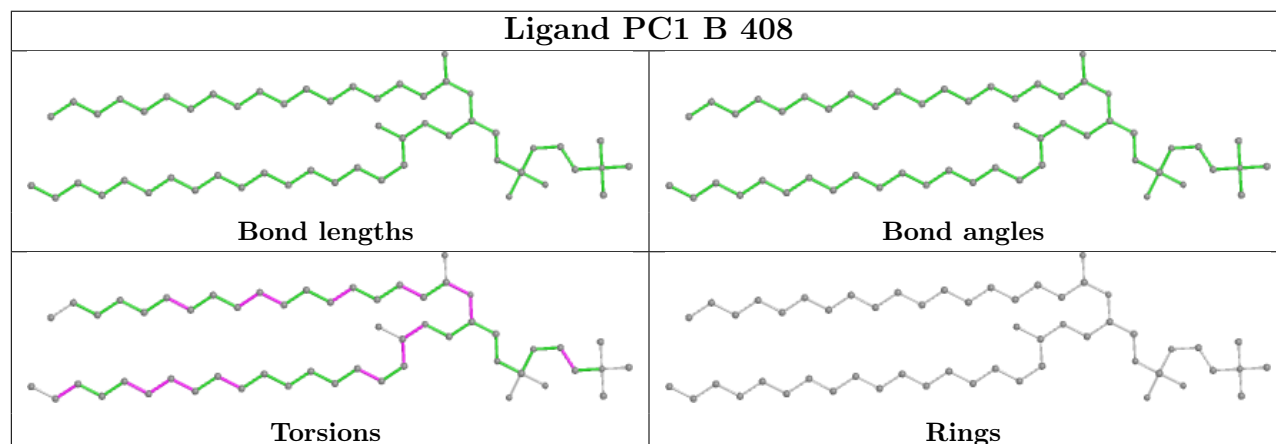
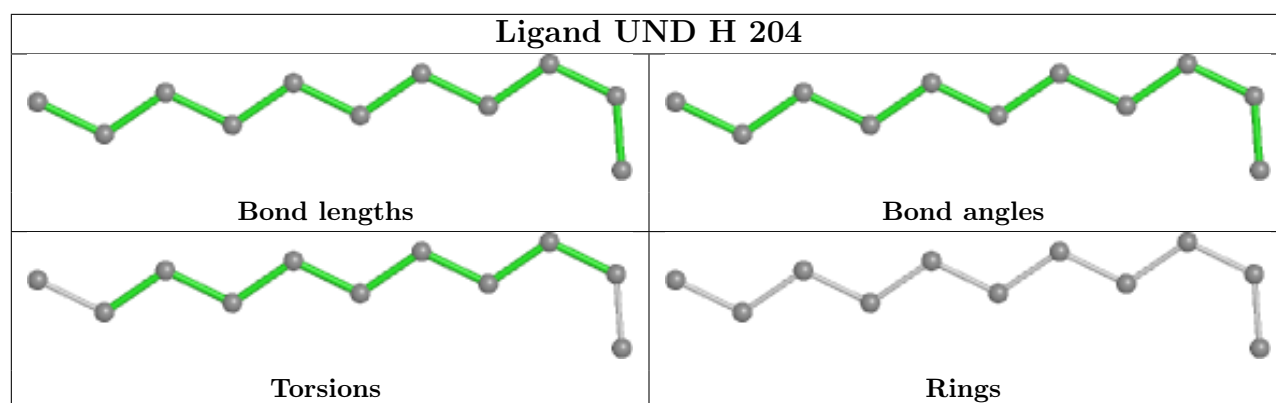


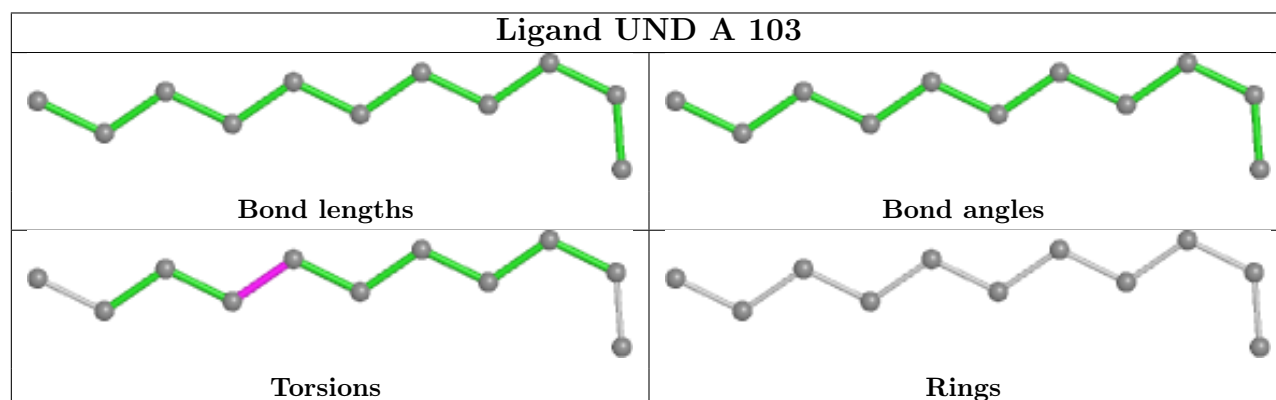
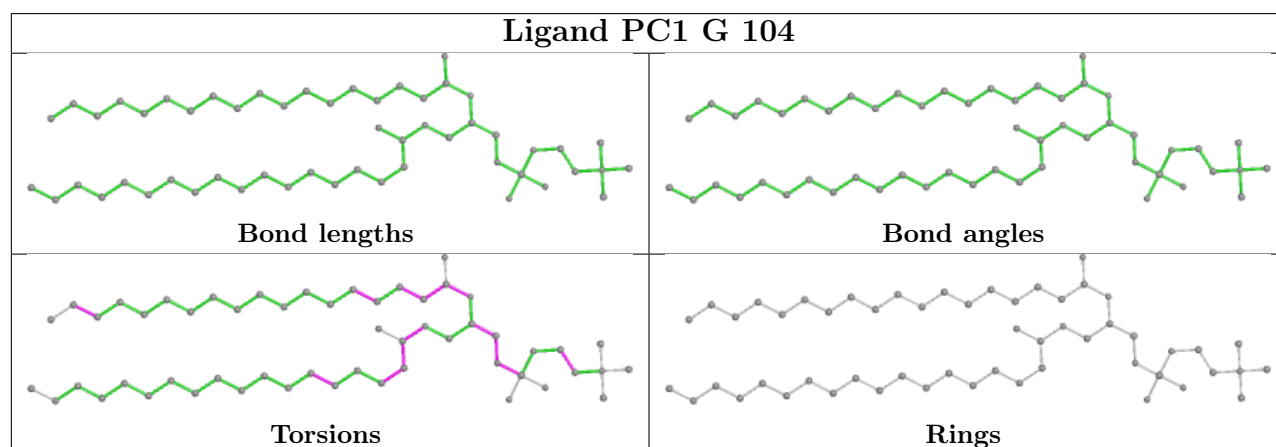
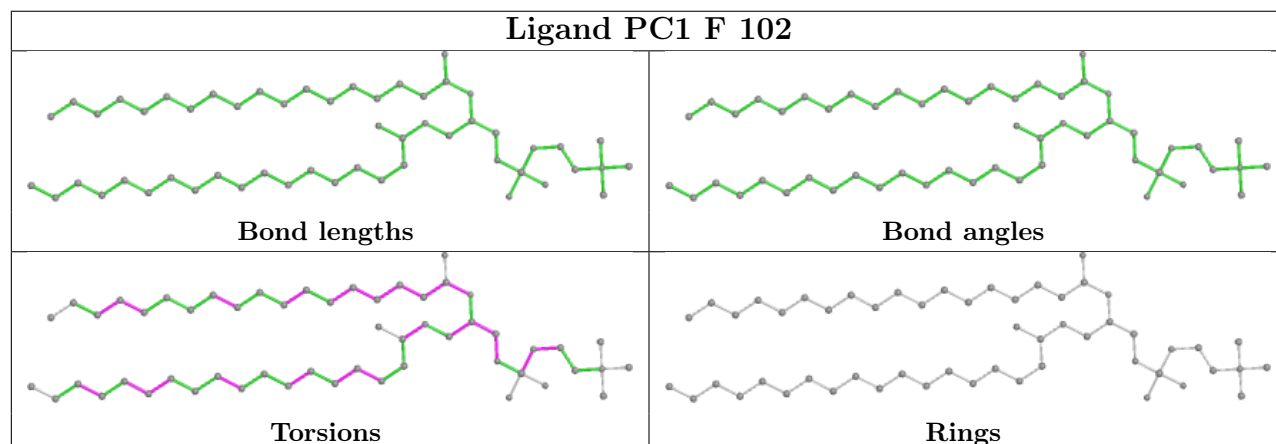
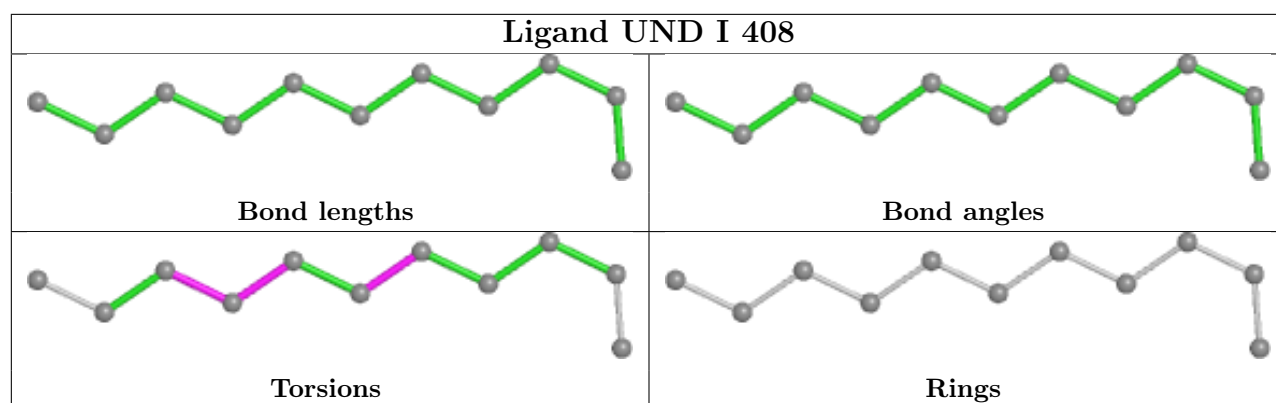


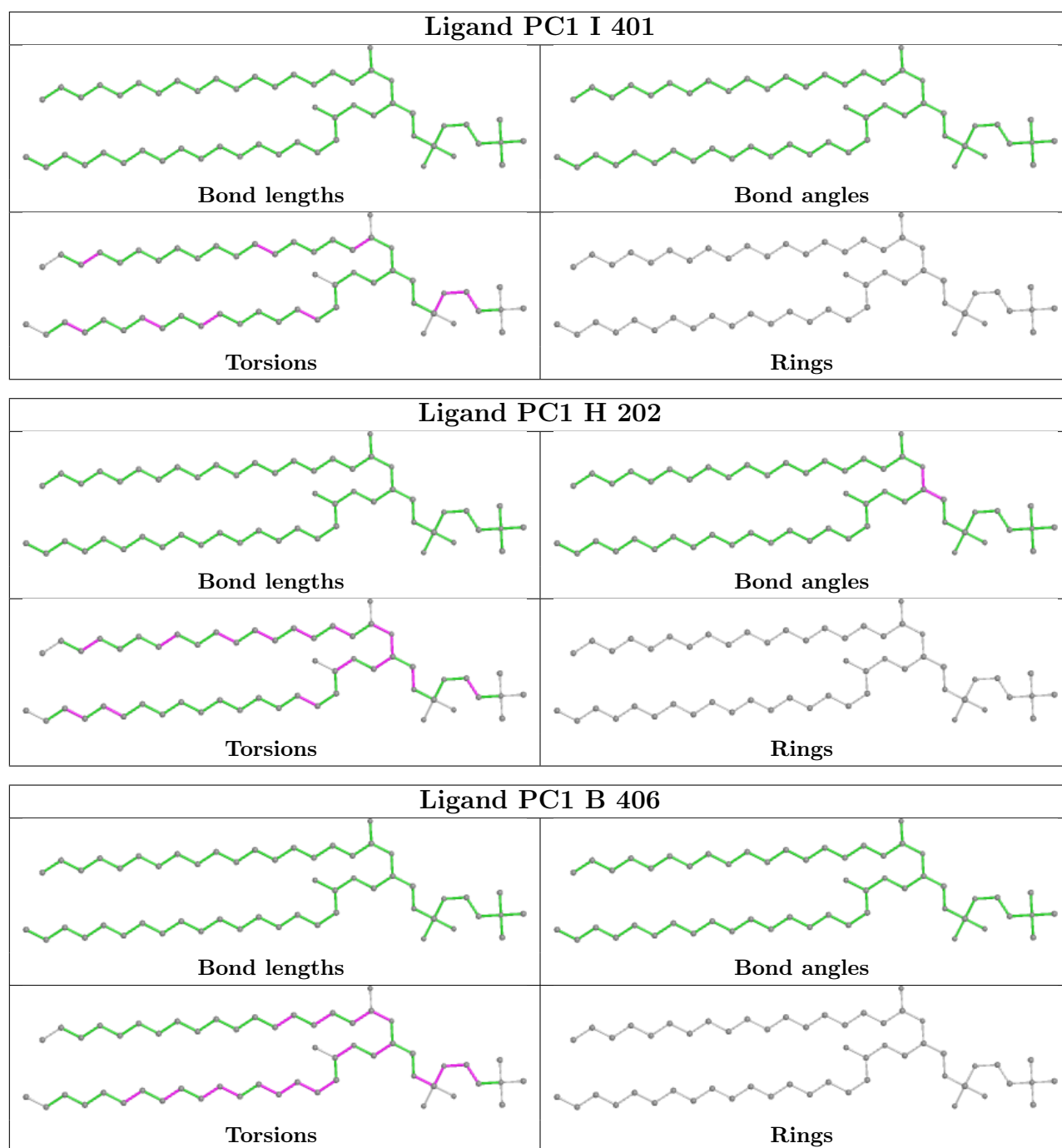


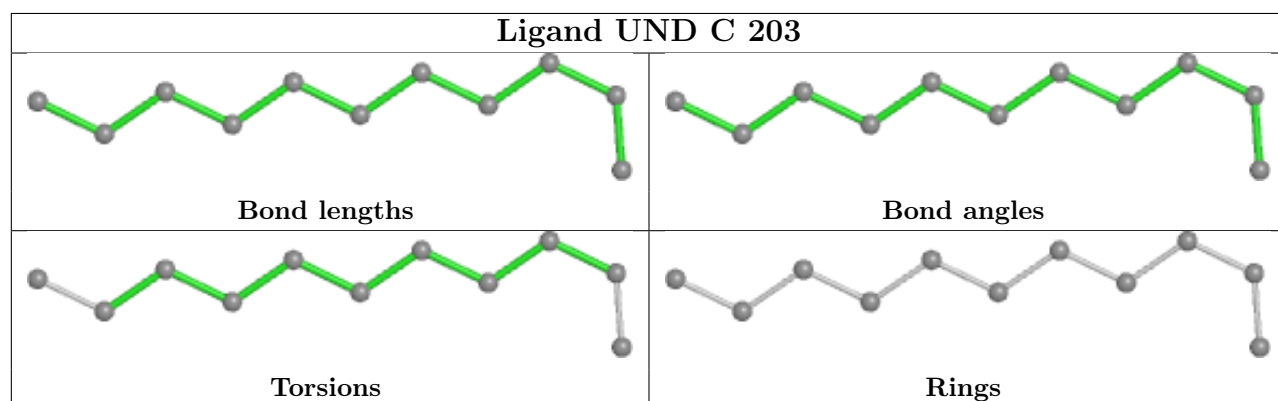
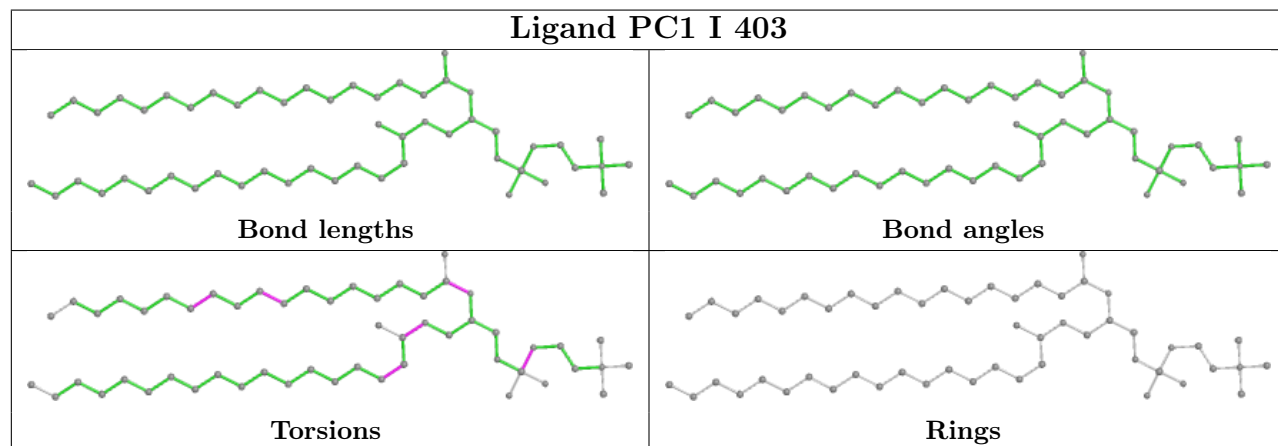
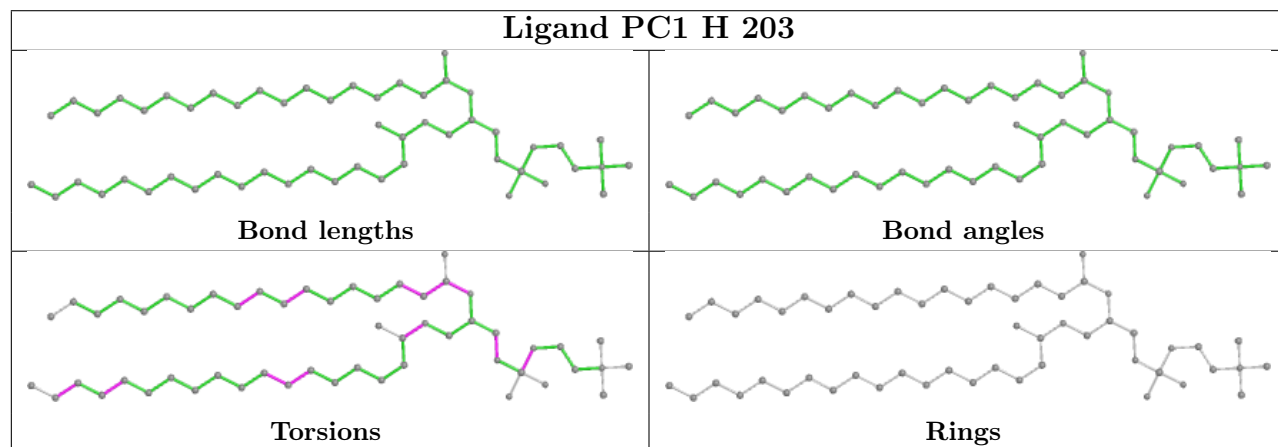
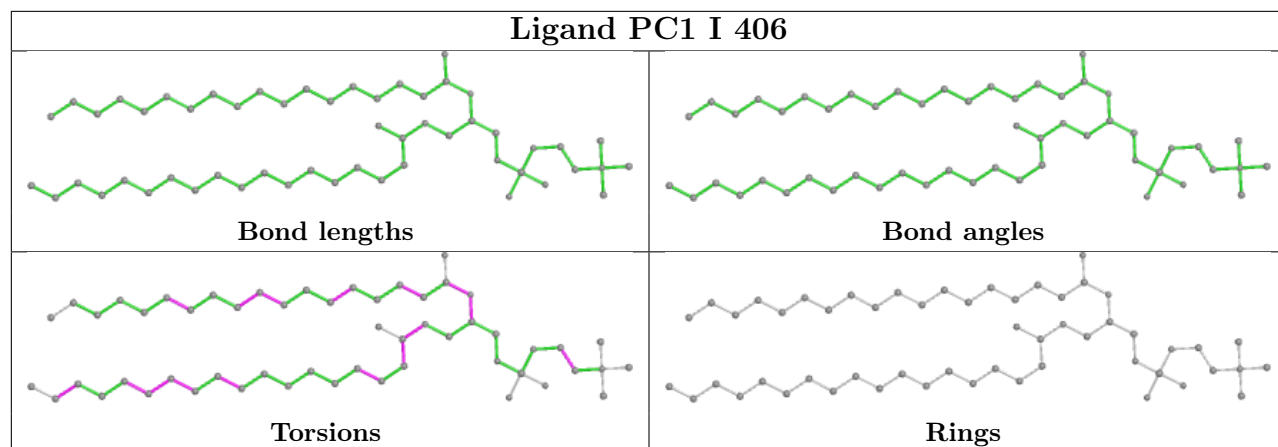


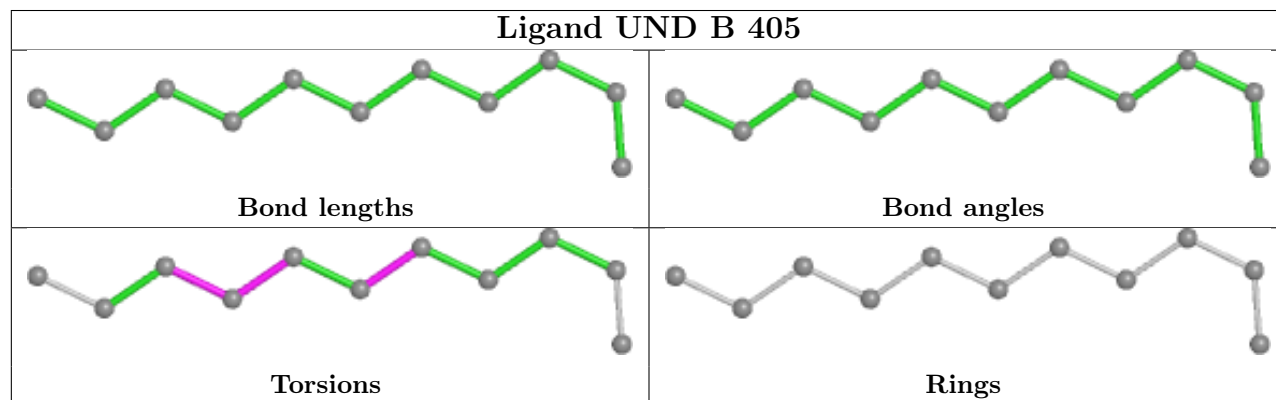
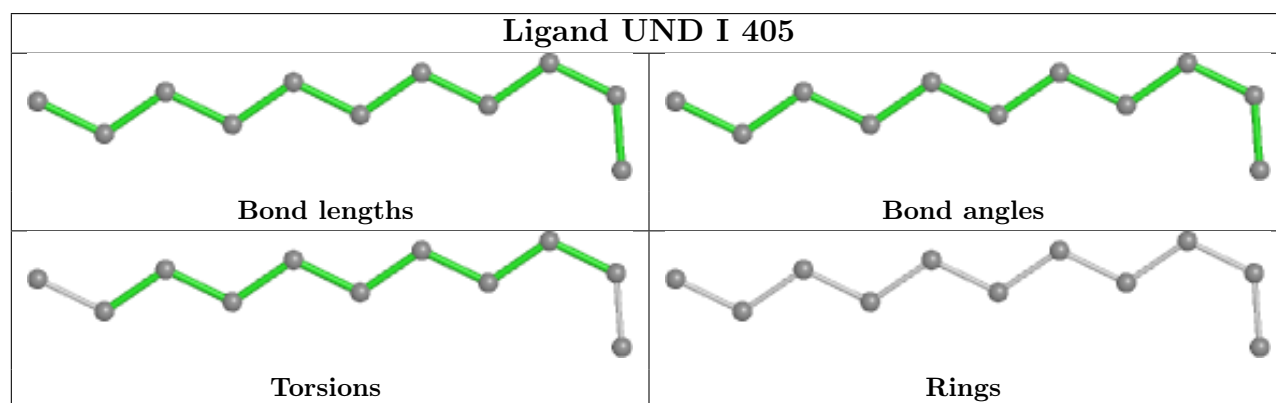
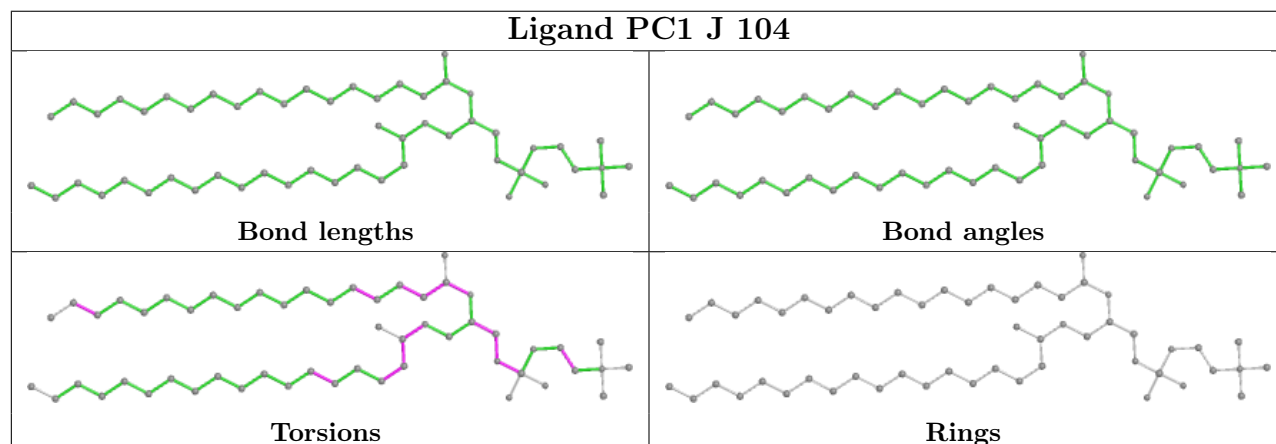
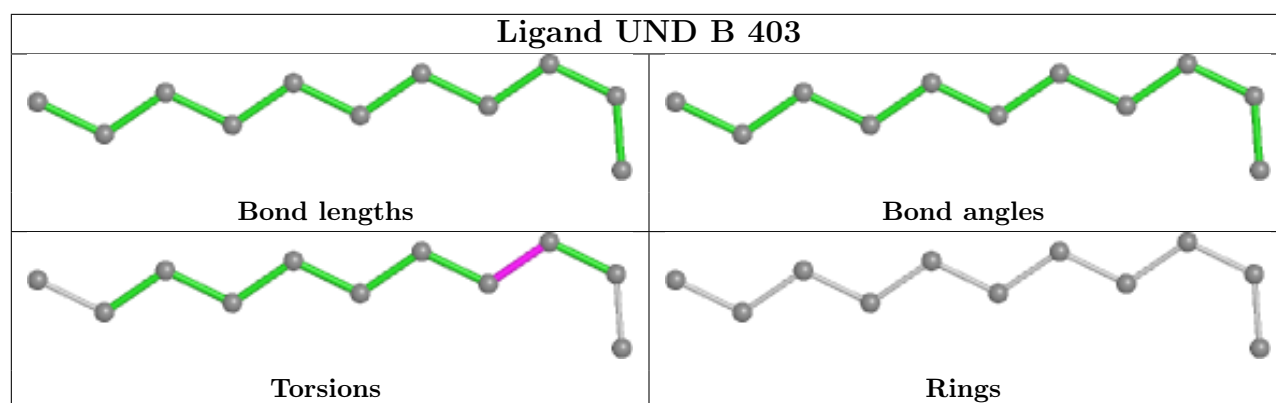


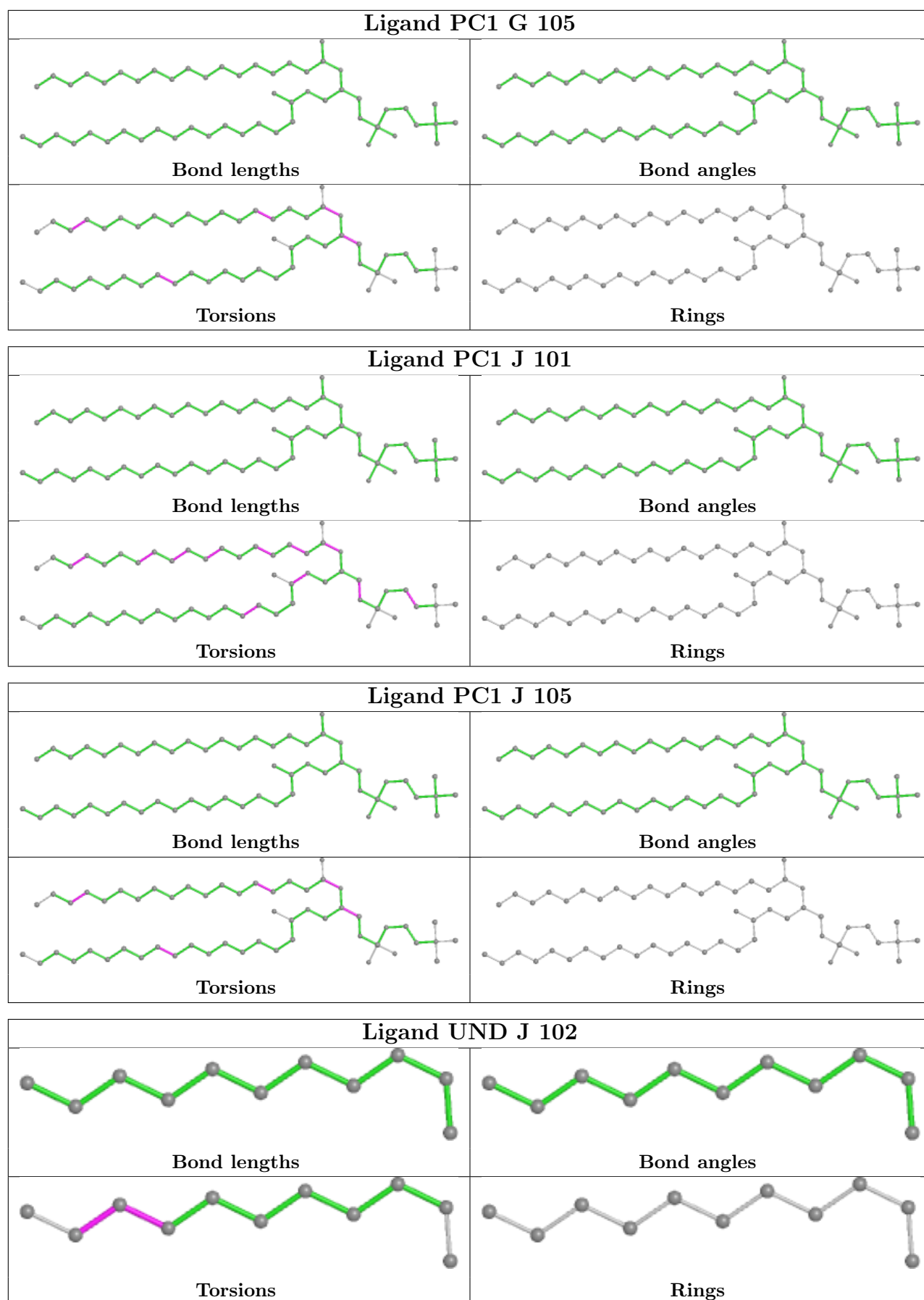


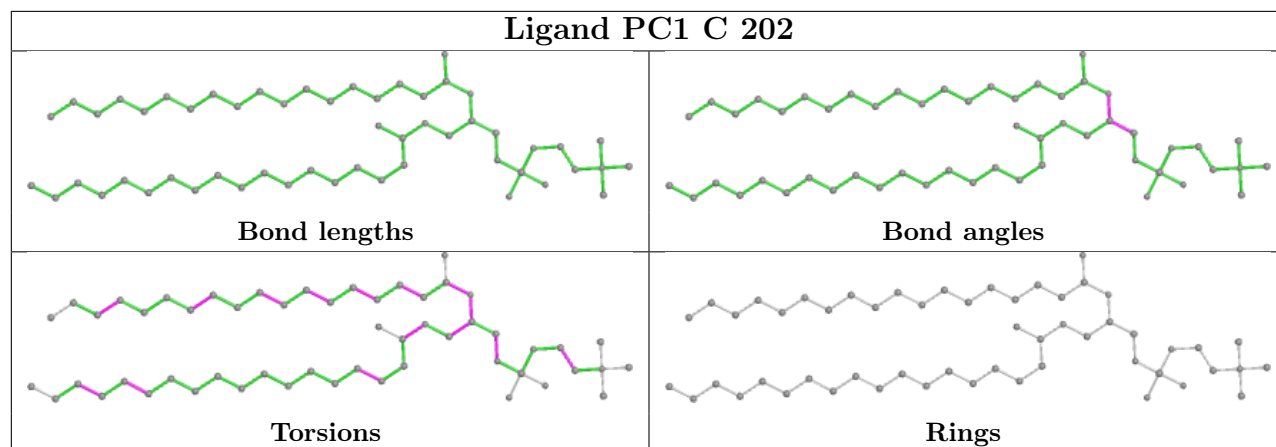












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

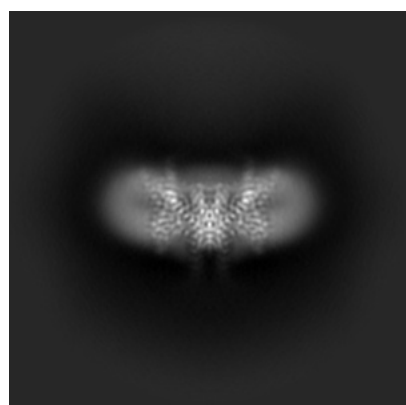
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31904. These allow visual inspection of the internal detail of the map and identification of artifacts.

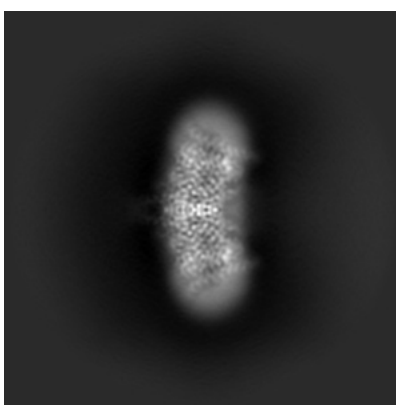
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

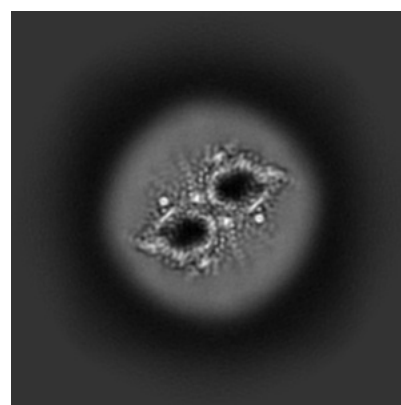
6.1.1 Primary map



X



Y

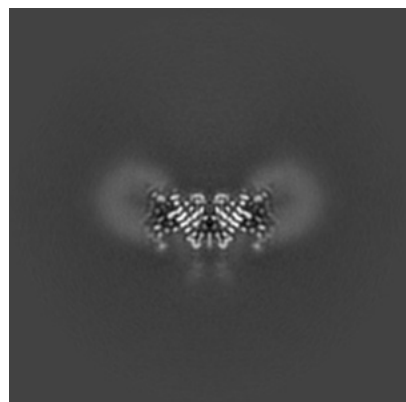


Z

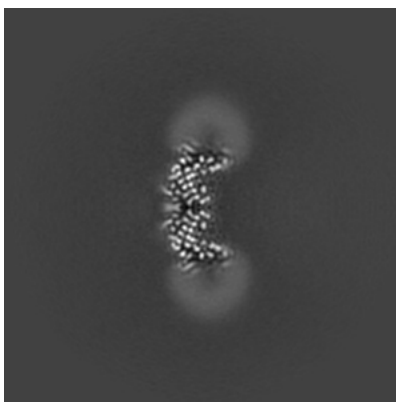
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

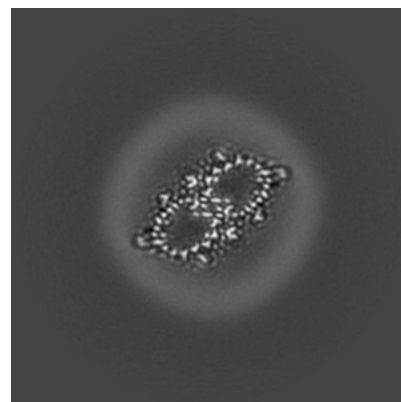
6.2.1 Primary map



X Index: 160



Y Index: 160

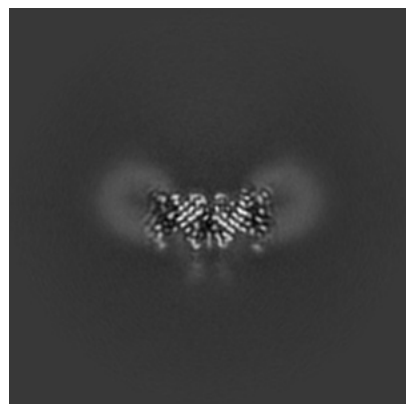


Z Index: 160

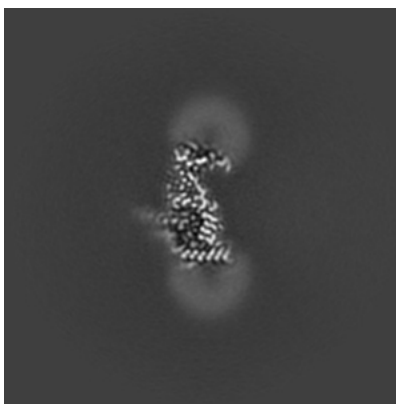
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

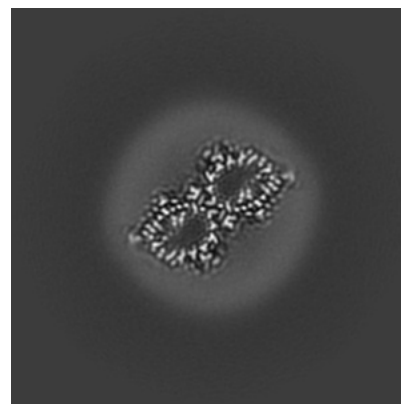
6.3.1 Primary map



X Index: 161



Y Index: 166



Z Index: 151

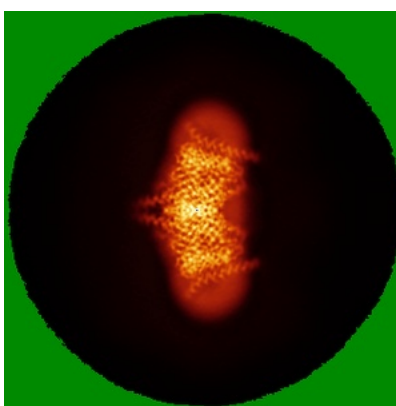
The images above show the largest variance slices of the map in three orthogonal directions.

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

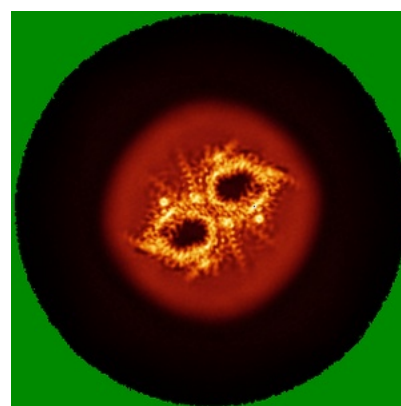
6.4.1 Primary map



X



Y

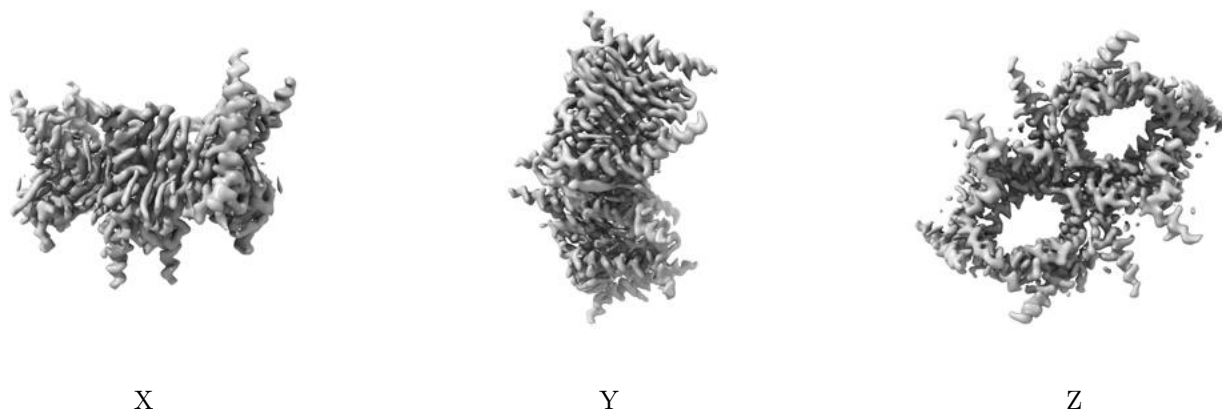


Z

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

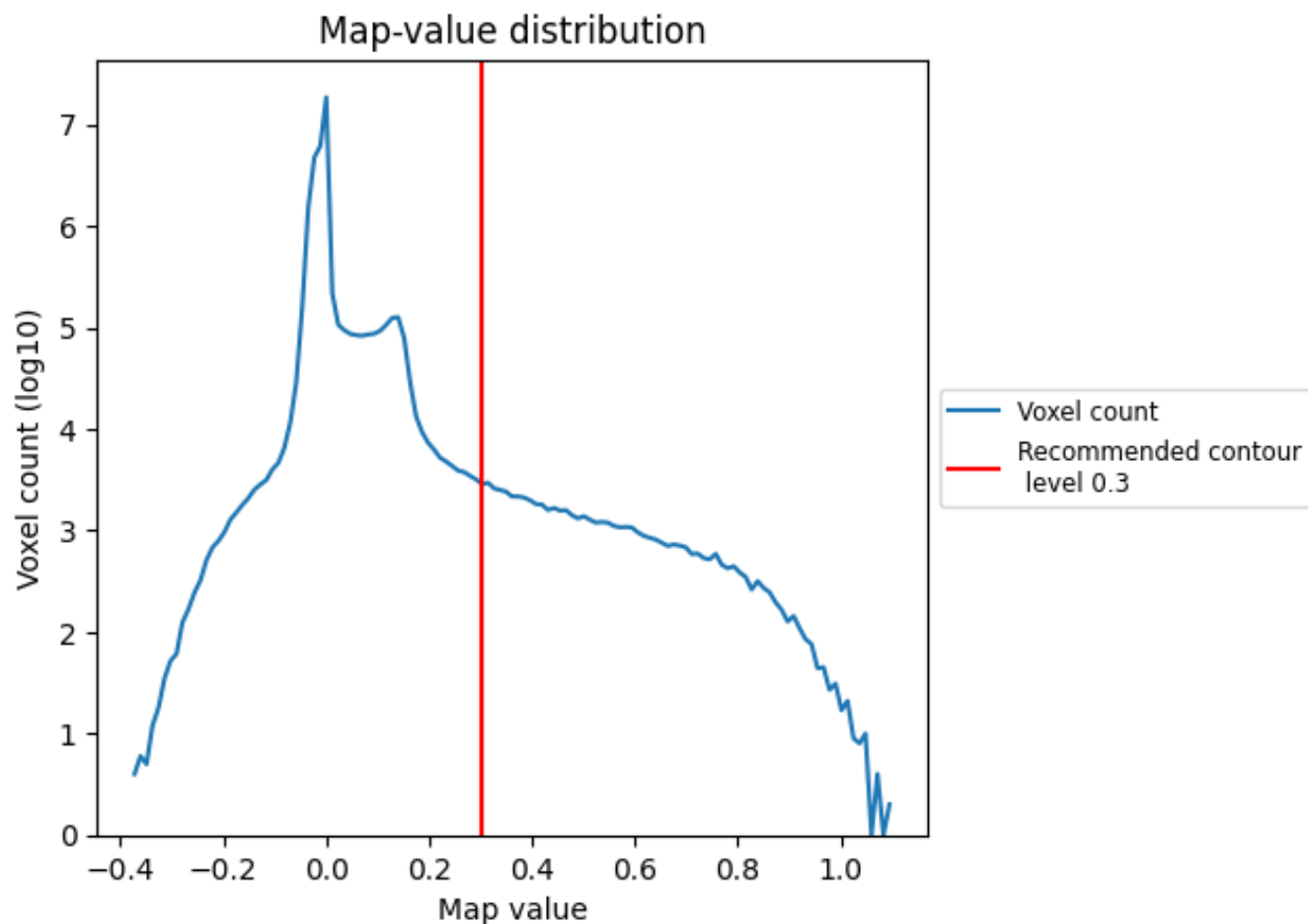
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

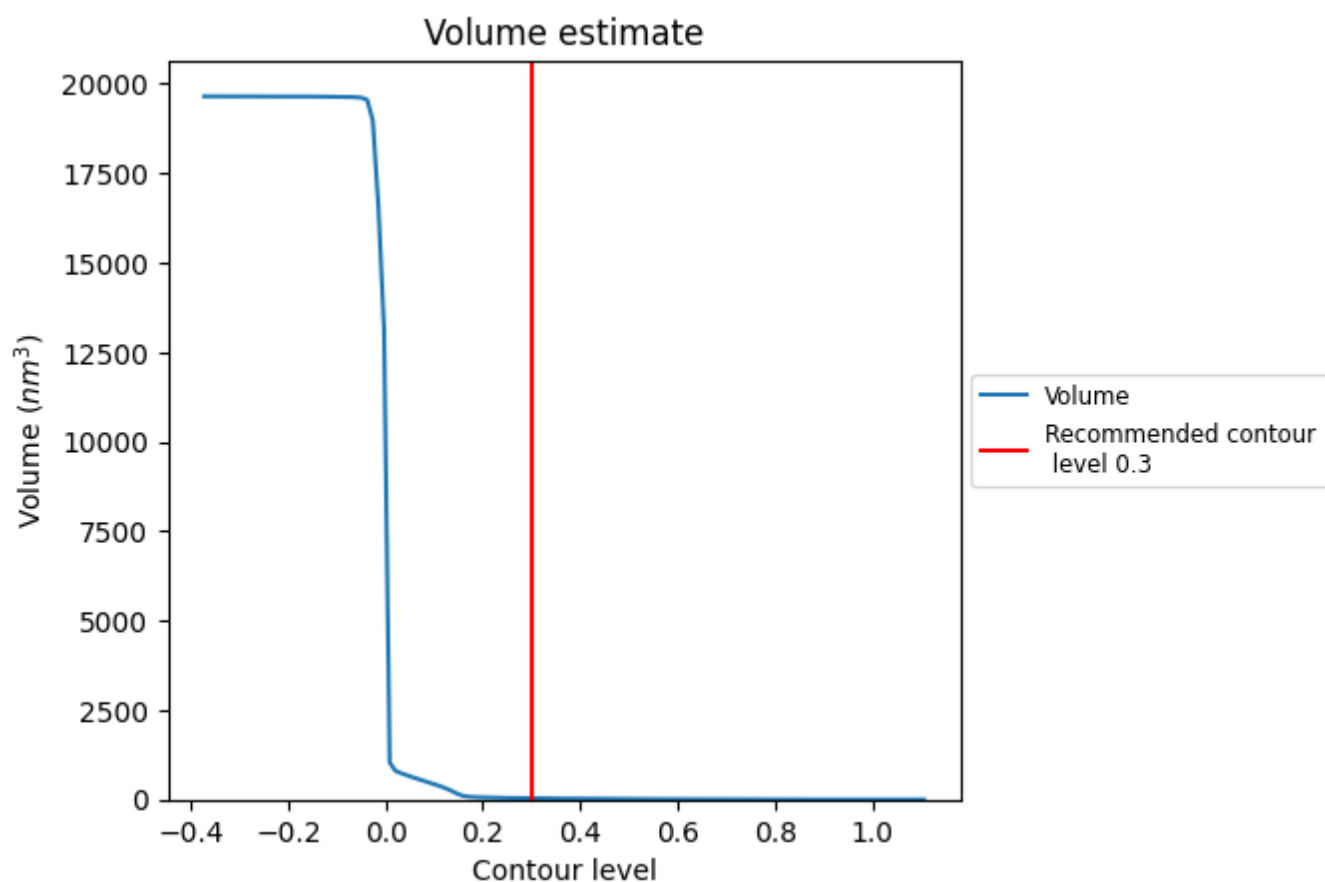
This section contains the results of statistical analysis of the map.

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.

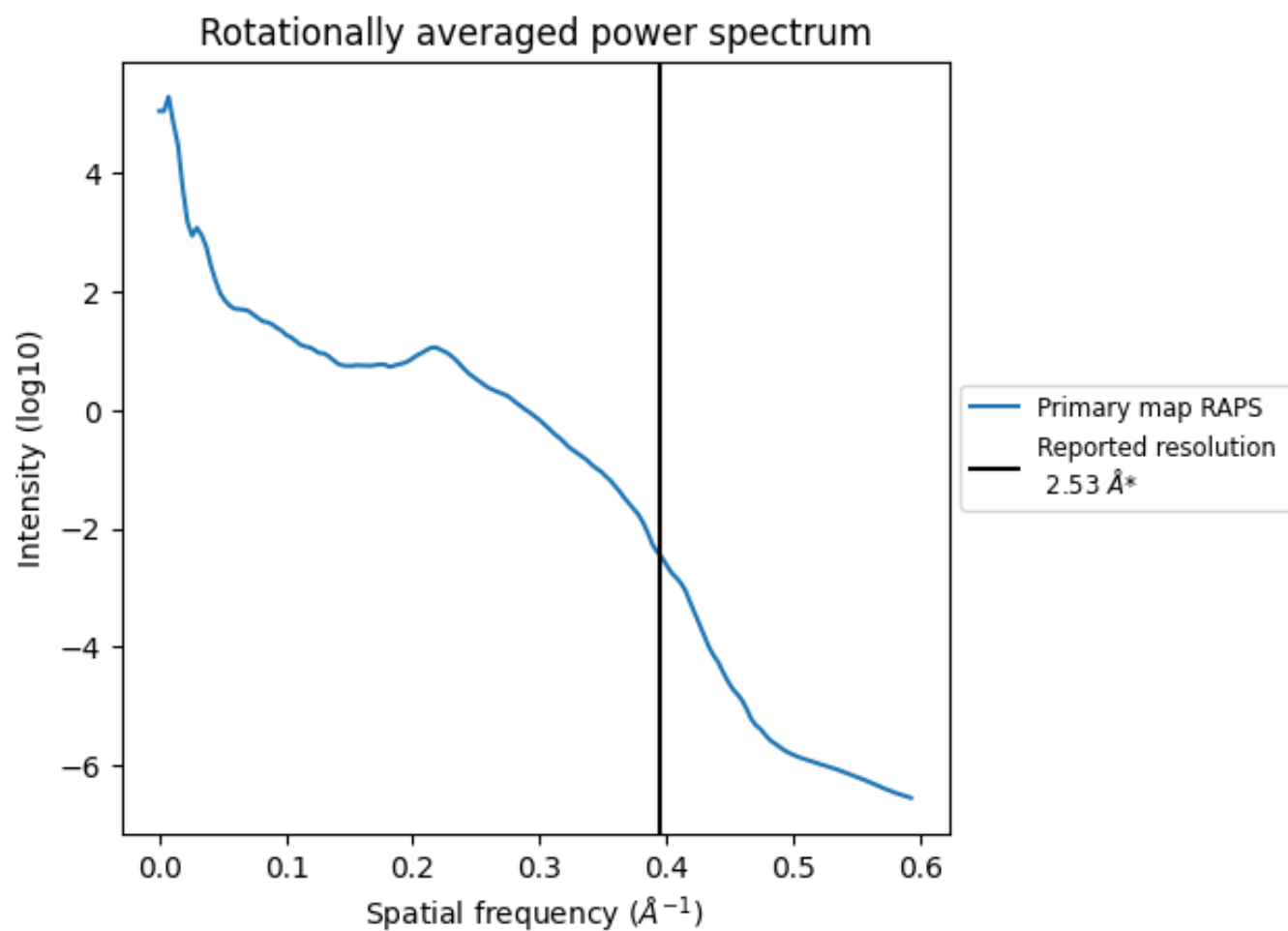
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 33 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 0.395 Å⁻¹

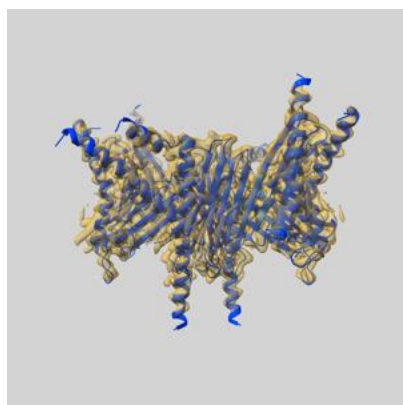
8 Fourier-Shell correlation

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

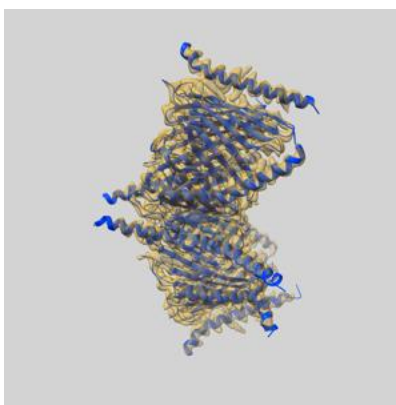
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31904 and PDB model 7VD2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

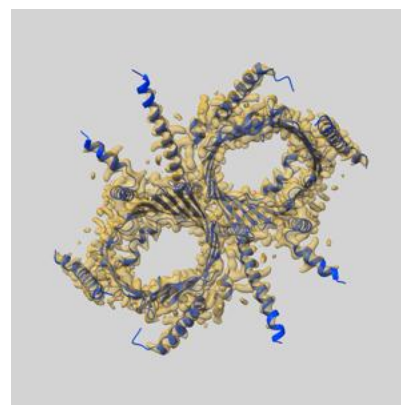
9.1 Map-model overlay [i](#)



X



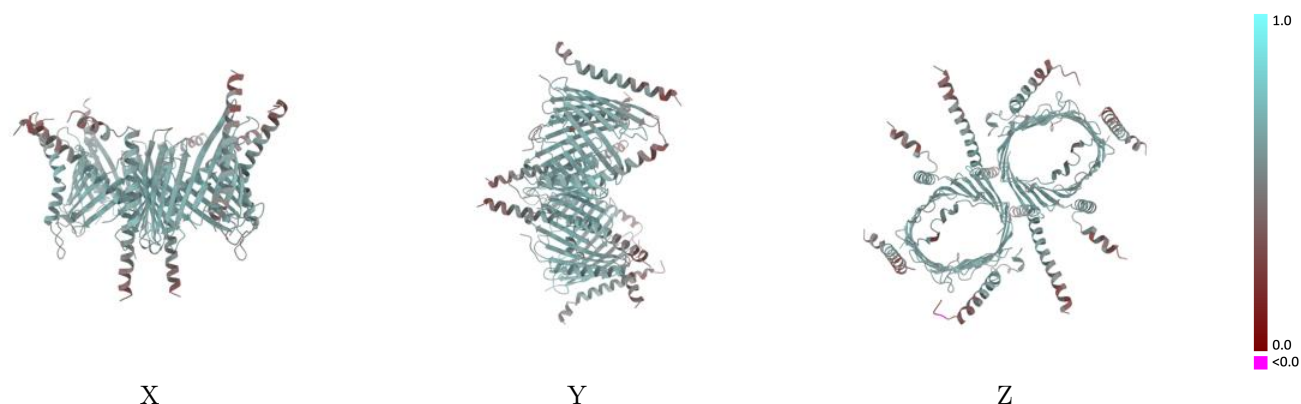
Y



Z

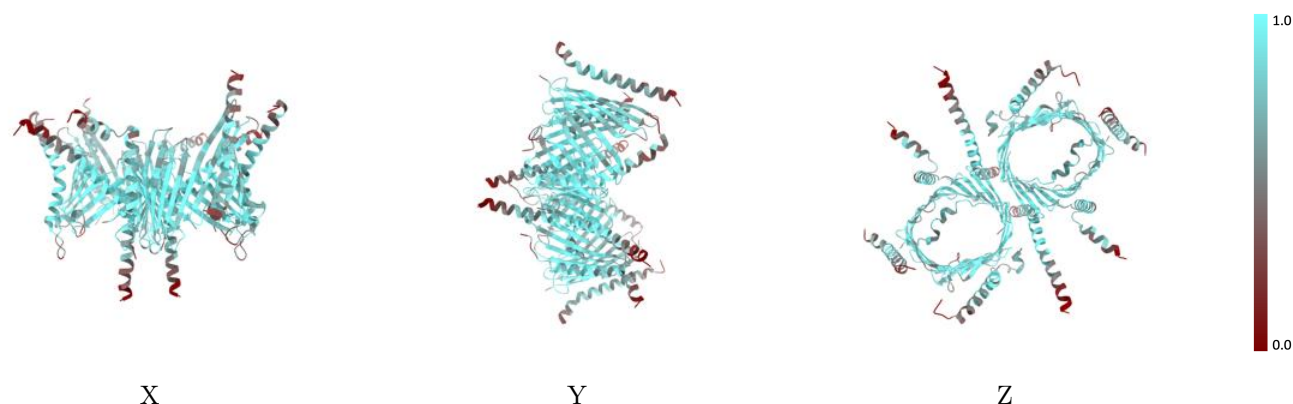
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



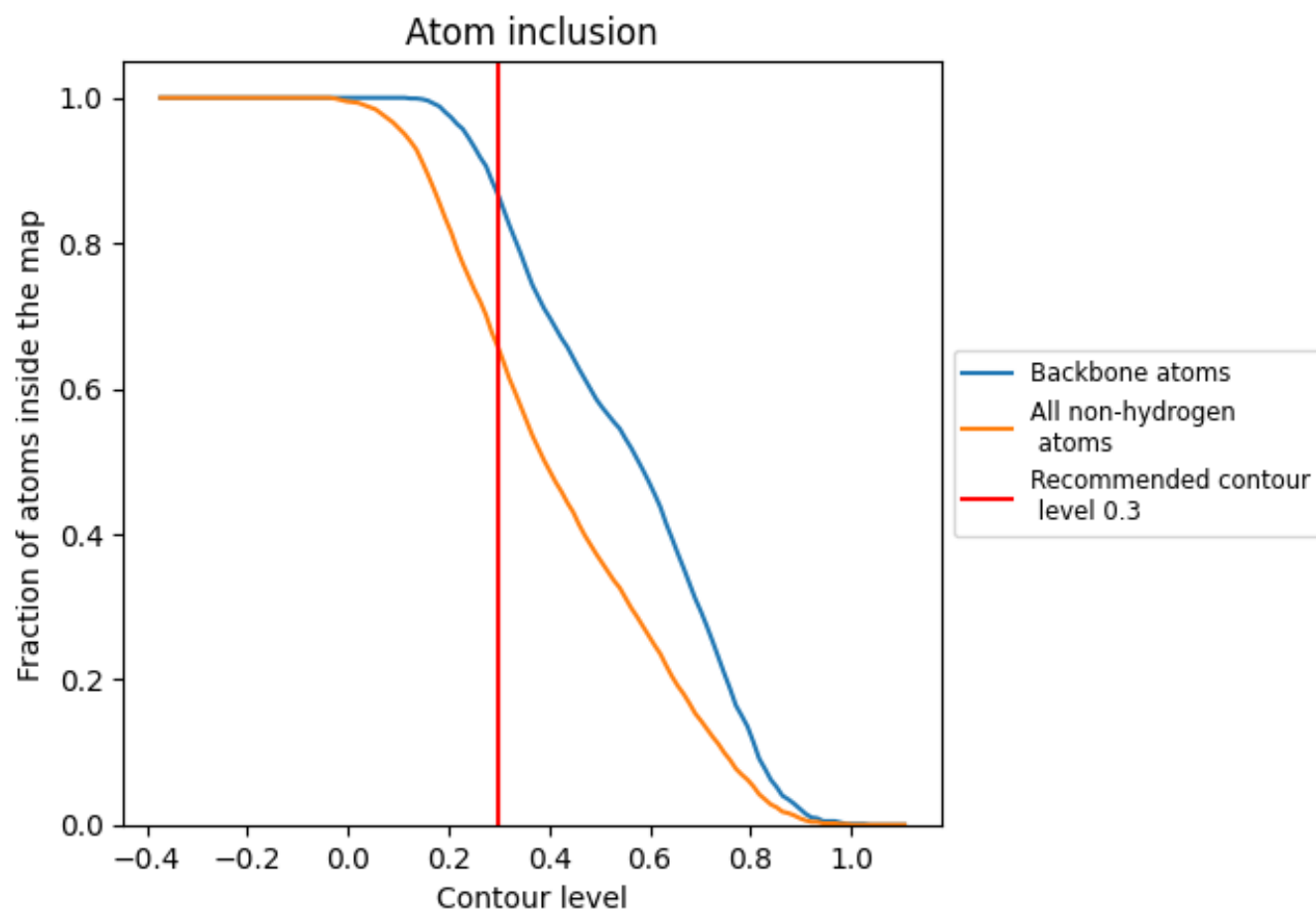
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 65% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6540	<div></div> 0.5380
A	<div></div> 0.5350	<div></div> 0.5220
B	<div></div> 0.7670	<div></div> 0.5810
C	<div></div> 0.4930	<div></div> 0.4830
D	<div></div> 0.5520	<div></div> 0.4770
E	<div></div> 0.5490	<div></div> 0.4680
F	<div></div> 0.5520	<div></div> 0.5280
G	<div></div> 0.4990	<div></div> 0.4680
H	<div></div> 0.4890	<div></div> 0.4820
I	<div></div> 0.7610	<div></div> 0.5820
J	<div></div> 0.4950	<div></div> 0.4610

