



## Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 01:26 PM JST

PDB ID : 7W77  
EMDB ID : EMD-32341  
Title : cryo-EM structure of human NaV1.3/beta1/beta2-bulleyaconitineA  
Authors : Jiang, D.; Li, X.  
Deposited on : 2021-12-03  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.39

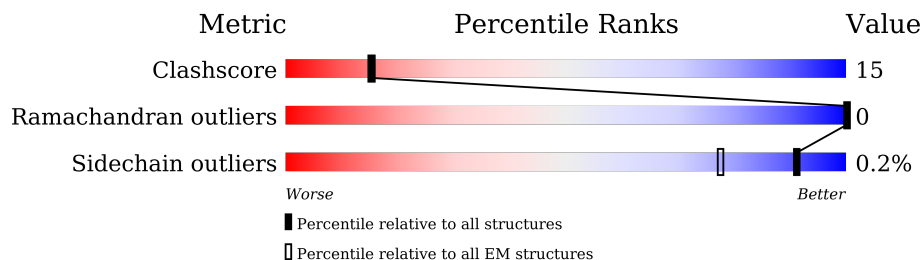
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	218	<div> <div>5%</div> <div>57%</div> <div>22%</div> <div>21%</div> </div>
2	C	215	<div> <div>46%</div> <div>36%</div> <div>21%</div> <div>43%</div> </div>
3	D	1951	<div> <div>5%</div> <div>41%</div> <div>17%</div> <div>42%</div> </div>
4	E	3	<div> <div>67%</div> <div>33%</div> </div>
5	F	2	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12051 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 Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 2 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	122	Total	C	N	O	S	4	0
			1007	630	178	188	11		

- Molecule 3 is a protein called Sodium channel protein type 3 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1129	Total	C	N	O	S	0	0
			9051	6013	1413	1547	78		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



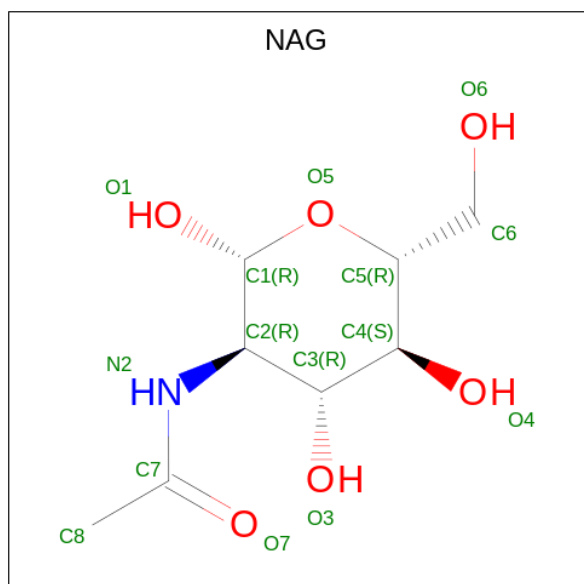
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



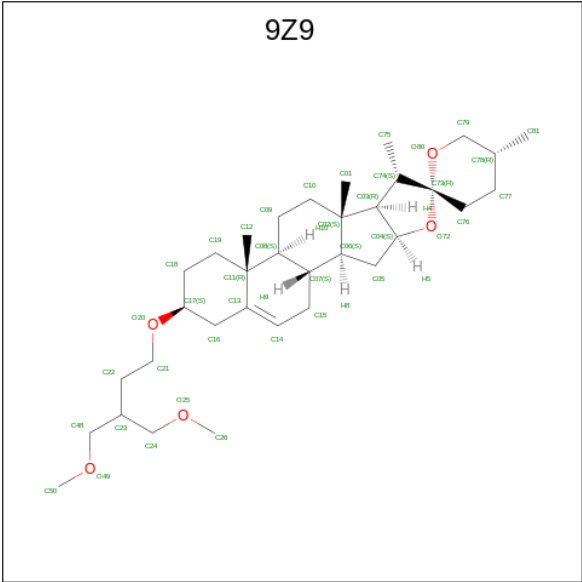
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

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



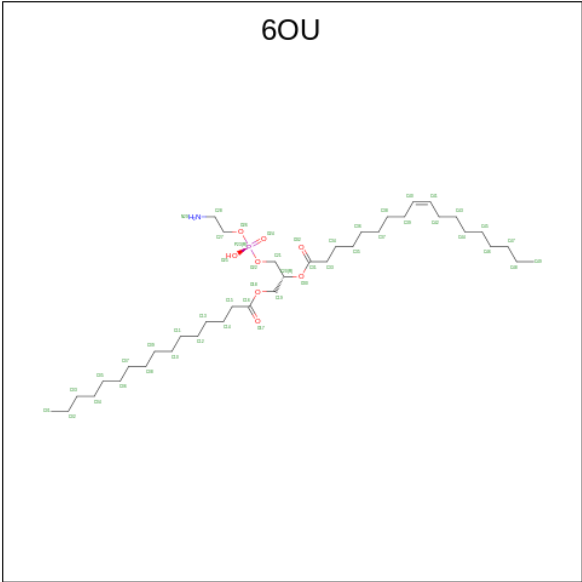
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula:  $C_{34}H_{56}O_5$ ).



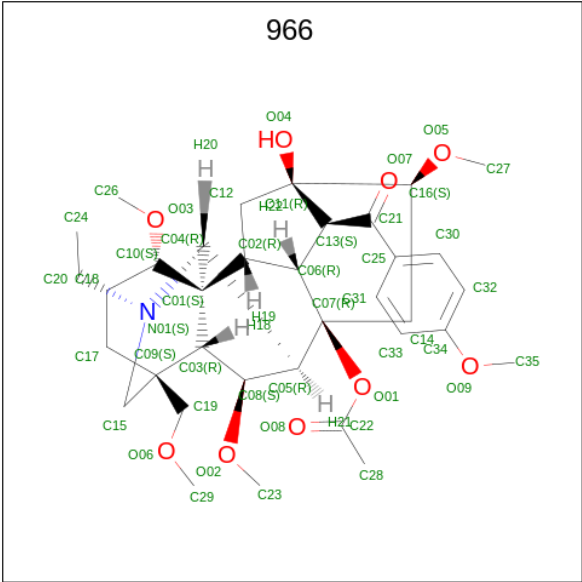
Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			32	29	3	
7	D	1	Total	C	O	0
			32	29	3	
7	D	1	Total	C	O	0
			32	29	3	

- Molecule 8 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	AltConf
8	D	1	Total C 9 9	0
8	D	1	Total C O P 37 28 8 1	0
8	D	1	Total C O 28 23 5	0
8	D	1	Total C N O P 33 23 1 8 1	0
8	D	1	Total C N O P 37 27 1 8 1	0
8	D	1	Total C O 27 23 4	0
8	D	1	Total C O 14 12 2	0
8	D	1	Total C O 14 12 2	0
8	D	1	Total C 11 11	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 13 11 2	0
8	D	1	Total C O 11 10 1	0

- Molecule 9 is [(1S,2R,3R,4R,5R,6S,8R,9S,13S,16S,17R,18R)-11-ethyl-5-hydroxy-6,16,18-trimethoxy-4-(4-methoxybenzoyl)-13-(methoxymethyl)-11-azahexacyclo[7.7.2.12,5.01,10.03,8.013,17]nonadecan-8-yl] acetate (three-letter code: 966) (formula: C<sub>35</sub>H<sub>49</sub>NO<sub>9</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			45	35	1	9	

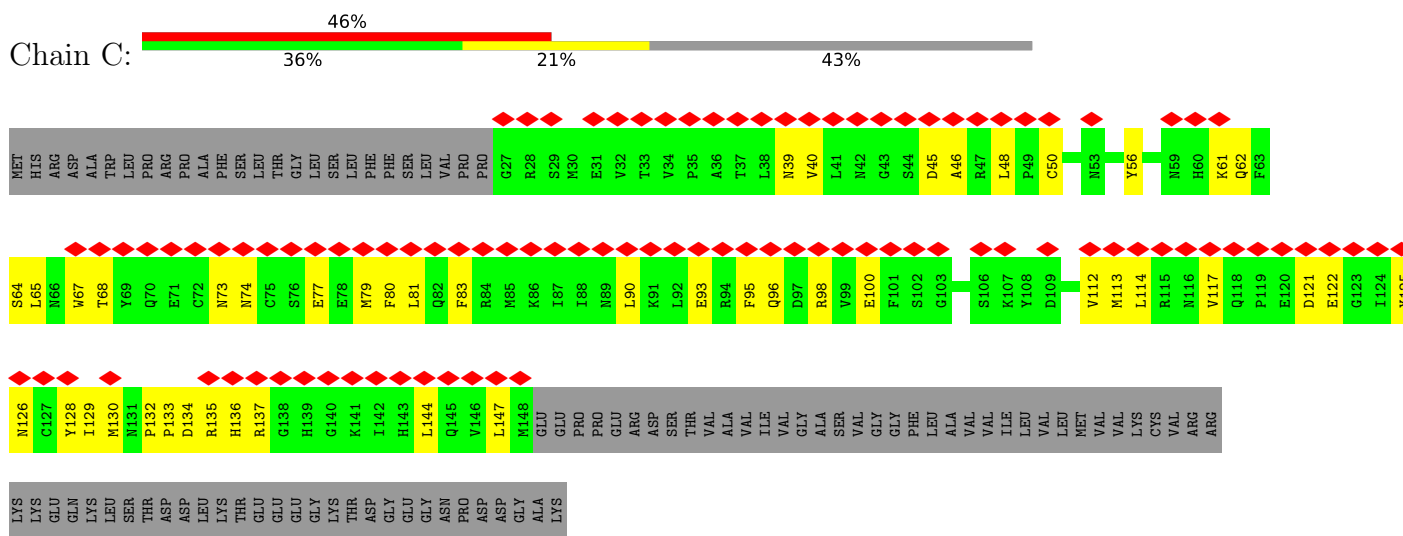
### 3 Residue-property plots

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

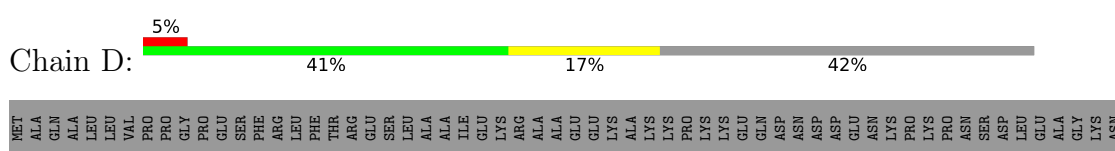
- Molecule 1: Sodium channel subunit beta-1



- Molecule 2: Sodium channel subunit beta-2



- Molecule 3: Sodium channel protein type 3 subunit alpha









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1403849	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 ( $e^-/\text{\AA}^2$ )	60	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	4.678	Depositor
Minimum map value	-3.653	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.417	Depositor
Map size ( $\text{\AA}$ )	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 6OU, 966, 9Z9

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	B	0.25	0/1442	0.51	0/1949
2	C	0.27	0/1041	0.58	1/1405 (0.1%)
3	D	0.26	0/9272	0.48	3/12572 (0.0%)
All	All	0.26	0/11755	0.50	4/15926 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1606	LEU	CA-CB-CG	7.84	133.34	115.30
3	D	1384	CYS	CB-CA-C	-7.46	95.49	110.40
3	D	180	LEU	CA-CB-CG	5.39	127.70	115.30
2	C	132	PRO	CA-N-CD	-5.24	104.16	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1382	SER	Mainchain

## 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	B	1416	0	1380	32	0
2	C	1007	0	978	31	0
3	D	9051	0	9239	233	0
4	E	39	0	34	0	0
5	F	28	0	25	0	0
6	B	56	0	52	1	0
6	D	14	0	13	0	0
7	D	96	0	0	55	0
8	D	299	0	0	0	0
9	D	45	0	0	0	0
All	All	12051	0	11721	347	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 15.

All (347) 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:D:2002:9Z9:C08	7:D:2002:9Z9:C11	1.76	1.63
7:D:2003:9Z9:C11	7:D:2003:9Z9:C08	1.76	1.62
7:D:2003:9Z9:C02	7:D:2003:9Z9:C03	1.76	1.57
7:D:2002:9Z9:C02	7:D:2002:9Z9:C03	1.77	1.57
7:D:2013:9Z9:C11	7:D:2013:9Z9:C08	1.75	1.57
7:D:2013:9Z9:C03	7:D:2013:9Z9:C02	1.76	1.56
7:D:2002:9Z9:C05	7:D:2002:9Z9:C04	1.82	1.53
7:D:2003:9Z9:C04	7:D:2003:9Z9:C05	1.82	1.53
7:D:2013:9Z9:C04	7:D:2013:9Z9:C05	1.83	1.52
7:D:2002:9Z9:C81	7:D:2002:9Z9:C78	1.91	1.48
7:D:2013:9Z9:C81	7:D:2013:9Z9:C78	1.91	1.46
7:D:2003:9Z9:C81	7:D:2003:9Z9:C78	1.91	1.46
3:D:1392:ARG:HE	3:D:1724:PRO:CG	1.70	1.04
3:D:1392:ARG:HH21	3:D:1724:PRO:HD2	1.17	1.03
7:D:2002:9Z9:C02	7:D:2002:9Z9:C74	2.46	0.94
7:D:2013:9Z9:C02	7:D:2013:9Z9:C74	2.44	0.93
7:D:2003:9Z9:C02	7:D:2003:9Z9:C74	2.45	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:2002:9Z9:C81	7:D:2002:9Z9:C79	2.51	0.88
3:D:756:ILE:HG22	3:D:757:VAL:N	1.88	0.88
3:D:1392:ARG:NH2	3:D:1724:PRO:HD2	1.88	0.87
3:D:1516:GLN:HE21	3:D:1578:VAL:HG13	1.42	0.85
3:D:1392:ARG:HE	3:D:1724:PRO:CD	1.90	0.85
7:D:2013:9Z9:C81	7:D:2013:9Z9:C79	2.52	0.84
7:D:2003:9Z9:C81	7:D:2003:9Z9:C79	2.52	0.84
7:D:2013:9Z9:C03	7:D:2013:9Z9:C06	2.57	0.82
3:D:756:ILE:HG22	3:D:757:VAL:H	1.44	0.81
3:D:358:ASN:HB2	3:D:362:GLY:HA2	1.62	0.80
7:D:2002:9Z9:C03	7:D:2002:9Z9:C06	2.61	0.79
7:D:2003:9Z9:C03	7:D:2003:9Z9:C06	2.61	0.78
3:D:267:GLN:OE1	3:D:1624:ARG:NH1	2.18	0.77
7:D:2013:9Z9:C81	7:D:2013:9Z9:C77	2.63	0.77
7:D:2002:9Z9:C81	7:D:2002:9Z9:C77	2.62	0.76
7:D:2002:9Z9:C03	7:D:2002:9Z9:C01	2.62	0.76
7:D:2003:9Z9:C81	7:D:2003:9Z9:C77	2.63	0.76
7:D:2002:9Z9:C02	7:D:2002:9Z9:C04	2.55	0.76
3:D:756:ILE:CG2	3:D:757:VAL:H	1.98	0.76
7:D:2003:9Z9:C03	7:D:2003:9Z9:C01	2.63	0.76
7:D:2013:9Z9:C03	7:D:2013:9Z9:C01	2.63	0.75
7:D:2003:9Z9:C04	7:D:2003:9Z9:C06	2.64	0.75
7:D:2002:9Z9:C04	7:D:2002:9Z9:C06	2.65	0.74
3:D:1516:GLN:NE2	3:D:1578:VAL:HG13	2.01	0.74
7:D:2013:9Z9:C04	7:D:2013:9Z9:C06	2.65	0.74
7:D:2013:9Z9:C11	7:D:2013:9Z9:C09	2.64	0.74
3:D:756:ILE:CG2	3:D:757:VAL:N	2.52	0.73
7:D:2002:9Z9:C08	7:D:2002:9Z9:C12	2.67	0.73
7:D:2003:9Z9:C11	7:D:2003:9Z9:C09	2.67	0.72
3:D:1683:GLU:HB2	3:D:1717:PRO:HB3	1.71	0.72
3:D:1338:VAL:HG21	3:D:1466:VAL:HG11	1.72	0.71
7:D:2002:9Z9:C11	7:D:2002:9Z9:C09	2.67	0.71
3:D:1413:VAL:HA	3:D:1419:TRP:HB3	1.71	0.71
7:D:2013:9Z9:C08	7:D:2013:9Z9:C12	2.67	0.71
7:D:2003:9Z9:C74	7:D:2003:9Z9:C01	2.69	0.71
7:D:2003:9Z9:C08	7:D:2003:9Z9:C12	2.66	0.71
7:D:2003:9Z9:C03	7:D:2003:9Z9:C10	2.63	0.70
3:D:1360:LYS:HB3	3:D:1429:SER:HB2	1.74	0.69
3:D:831:ILE:HD11	3:D:854:ARG:HA	1.73	0.69
3:D:1392:ARG:NE	3:D:1724:PRO:CG	2.51	0.68
3:D:1743:ASN:HB3	3:D:1746:VAL:HG12	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:HB3	1:B:146:VAL:HG12	1.76	0.68
1:B:35:THR:HG22	1:B:109:THR:HA	1.76	0.68
3:D:253:LEU:HD13	3:D:1641:ILE:HG23	1.75	0.68
3:D:1193:TRP:HE1	3:D:1197:LYS:HE2	1.59	0.68
3:D:1602:VAL:O	3:D:1606:LEU:HD12	1.94	0.68
7:D:2002:9Z9:C74	7:D:2002:9Z9:C01	2.72	0.67
7:D:2013:9Z9:C03	7:D:2013:9Z9:C10	2.62	0.67
1:B:92:TRP:O	1:B:96:ARG:NH2	2.27	0.67
3:D:1431:ASP:HB3	3:D:1434:LEU:HD12	1.78	0.66
1:B:53:THR:OG1	1:B:125:ARG:NH1	2.29	0.66
3:D:1268:PHE:O	3:D:1274:TRP:NE1	2.27	0.65
7:D:2002:9Z9:C03	7:D:2002:9Z9:C10	2.64	0.65
3:D:1516:GLN:HG2	3:D:1578:VAL:CG1	2.27	0.65
2:C:113:MET:HE3	2:C:114:LEU:H	1.60	0.65
3:D:1392:ARG:HE	3:D:1724:PRO:HG3	1.61	0.65
3:D:408:ILE:HA	3:D:412:SER:HB3	1.77	0.65
3:D:1437:VAL:HB	3:D:1440:GLU:HB2	1.77	0.65
3:D:185:PHE:HD2	3:D:191:ASN:HB3	1.61	0.65
3:D:418:LEU:HD13	3:D:1644:LEU:HD23	1.77	0.65
1:B:21:CYS:SG	1:B:102:GLN:NE2	2.71	0.64
3:D:218:PHE:O	3:D:222:ARG:N	2.26	0.64
7:D:2003:9Z9:C09	7:D:2003:9Z9:C12	2.75	0.64
3:D:253:LEU:HB2	3:D:1641:ILE:HG12	1.79	0.64
2:C:134:ASP:OD1	2:C:135:ARG:N	2.31	0.64
1:B:24:VAL:HG22	1:B:41:ILE:HD12	1.79	0.63
3:D:1392:ARG:NE	3:D:1724:PRO:CD	2.60	0.62
1:B:61:GLN:NE2	1:B:114:ASN:O	2.25	0.62
3:D:379:LEU:HD23	3:D:385:TRP:HB2	1.80	0.62
3:D:142:CYS:SG	3:D:226:THR:OG1	2.57	0.62
3:D:961:LEU:O	3:D:965:MET:HG2	2.00	0.61
7:D:2013:9Z9:C08	7:D:2013:9Z9:C19	2.78	0.61
3:D:1464:ILE:O	3:D:1468:ILE:HG13	2.01	0.60
7:D:2002:9Z9:C11	7:D:2002:9Z9:C07	2.55	0.60
7:D:2013:9Z9:C74	7:D:2013:9Z9:C01	2.79	0.60
7:D:2002:9Z9:C12	7:D:2002:9Z9:C09	2.78	0.60
3:D:414:TYR:CZ	3:D:1648:LEU:HB2	2.37	0.60
3:D:1193:TRP:NE1	3:D:1197:LYS:HE2	2.16	0.60
3:D:1331:ALA:HA	3:D:1470:ASN:HD21	1.66	0.60
1:B:59:PHE:HZ	1:B:85:ARG:HE	1.50	0.59
3:D:1682:LYS:HE3	3:D:1691:ASN:HD22	1.68	0.59
1:B:118:ASP:OD1	1:B:143:HIS:ND1	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:858:VAL:HB	3:D:1348:ILE:HD11	1.84	0.58
3:D:1558:LEU:O	3:D:1562:ASN:ND2	2.35	0.58
3:D:1479:GLY:N	3:D:1480:GLY:HA3	2.18	0.58
2:C:64:SER:HB3	2:C:130:MET:HB3	1.85	0.58
3:D:849:VAL:HG13	3:D:1356:LEU:HD21	1.85	0.58
3:D:1281:ASP:O	3:D:1285:VAL:HG23	2.03	0.58
3:D:176:ARG:HB2	3:D:184:THR:HB	1.85	0.58
7:D:2003:9Z9:C08	7:D:2003:9Z9:C19	2.79	0.58
7:D:2002:9Z9:C08	7:D:2002:9Z9:C19	2.79	0.57
2:C:95:PHE:HE2	2:C:121:ASP:HA	1.69	0.57
3:D:401:MET:SD	3:D:1700:ILE:HG22	2.45	0.57
3:D:406:LEU:O	3:D:410:LEU:N	2.37	0.57
2:C:128:TYR:HD2	2:C:137:ARG:HD3	1.68	0.57
3:D:757:VAL:HB	3:D:760:PRO:HG2	1.87	0.57
3:D:1427:VAL:HG12	3:D:1439:GLU:HA	1.86	0.57
3:D:808:VAL:HA	3:D:811:ILE:HG12	1.86	0.57
3:D:1213:VAL:HG22	3:D:1317:ARG:HB3	1.87	0.56
2:C:79:MET:SD	2:C:81:LEU:N	2.78	0.56
1:B:31:VAL:HG23	1:B:34:MET:HB2	1.86	0.56
3:D:1597:VAL:O	3:D:1601:ILE:HG12	2.05	0.56
3:D:1620:PHE:HE1	3:D:1624:ARG:HE	1.53	0.56
1:B:103:ASP:HB2	3:D:1733:PRO:HG3	1.87	0.56
3:D:250:VAL:HG21	3:D:422:VAL:HG21	1.87	0.56
3:D:404:PHE:HA	3:D:407:VAL:HG12	1.87	0.56
3:D:1541:VAL:O	3:D:1545:VAL:HG23	2.06	0.55
3:D:1315:LEU:HD22	3:D:1325:VAL:HG21	1.89	0.55
3:D:1638:ALA:HB1	3:D:1641:ILE:HD12	1.88	0.55
3:D:394:ARG:NH2	3:D:1687:ASP:OD2	2.39	0.55
3:D:1220:SER:HB2	3:D:1667:PHE:HE2	1.72	0.55
3:D:336:LEU:HD23	3:D:395:ALA:HB2	1.89	0.54
3:D:336:LEU:HD11	3:D:359:PRO:HG3	1.88	0.54
2:C:122:GLU:HA	2:C:144:LEU:O	2.08	0.54
3:D:263:LEU:O	3:D:267:GLN:HG2	2.07	0.54
3:D:1392:ARG:NE	3:D:1724:PRO:HG3	2.19	0.54
3:D:753:VAL:HG11	3:D:812:ILE:HD11	1.89	0.54
3:D:911:CYS:HB2	3:D:954:VAL:HG13	1.88	0.54
3:D:424:ALA:O	3:D:428:GLU:HG2	2.08	0.54
1:B:74:GLU:HG2	1:B:75:ASN:H	1.73	0.53
1:B:174:LEU:HD11	3:D:1257:LEU:HD21	1.90	0.53
7:D:2003:9Z9:C02	7:D:2003:9Z9:C04	2.55	0.53
3:D:820:PHE:HD1	3:D:826:ILE:HG13	1.74	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:832:VAL:O	3:D:836:LEU:HG	2.09	0.52
3:D:835:SER:O	3:D:838:GLU:HG3	2.09	0.52
3:D:1731:ILE:HD12	3:D:1738:LYS:HE2	1.91	0.52
2:C:65:LEU:HB3	2:C:83:PHE:HB3	1.91	0.52
2:C:67:TRP:CZ3	2:C:125:TYR:HB3	2.45	0.52
3:D:982:LEU:HB3	3:D:1461:ASN:ND2	2.25	0.52
3:D:1229:TYR:O	3:D:1232:GLN:HG2	2.10	0.51
3:D:962:ILE:O	3:D:966:LEU:HD23	2.10	0.51
1:B:42:SER:OG	1:B:125:ARG:NH2	2.42	0.51
2:C:48:LEU:HB3	2:C:112:VAL:HG23	1.92	0.51
3:D:1453:ILE:O	3:D:1457:PHE:HB3	2.09	0.51
3:D:376:LEU:HD21	3:D:403:PHE:HZ	1.75	0.51
3:D:1417:LYS:HG3	3:D:1708:SER:O	2.11	0.51
2:C:39:ASN:HB2	2:C:147:LEU:HD23	1.92	0.51
3:D:135:MET:SD	3:D:230:ILE:HG22	2.51	0.51
2:C:114:LEU:HD22	2:C:117:VAL:HG22	1.92	0.50
3:D:360:ASN:HB2	3:D:364:THR:HG22	1.93	0.50
3:D:1543:MET:HG2	3:D:1627:ARG:NH2	2.26	0.50
3:D:1392:ARG:HE	3:D:1724:PRO:HG2	1.66	0.50
3:D:1651:SER:HB2	3:D:1772:GLU:HG2	1.92	0.50
3:D:378:ARG:HD2	3:D:945:ILE:HD13	1.93	0.50
3:D:1680:VAL:HG11	3:D:1718:ILE:HG12	1.92	0.50
3:D:1375:ILE:HG21	3:D:1437:VAL:HG22	1.93	0.50
3:D:1546:GLU:OE1	3:D:1550:GLN:NE2	2.36	0.49
1:B:60:ARG:HG2	1:B:118:ASP:HB2	1.93	0.49
3:D:1543:MET:SD	3:D:1627:ARG:HB3	2.52	0.49
7:D:2013:9Z9:C11	7:D:2013:9Z9:C07	2.56	0.49
1:B:59:PHE:HE2	1:B:61:GLN:HE21	1.60	0.49
3:D:1215:MET:HE1	3:D:1250:ILE:HD13	1.95	0.49
3:D:1392:ARG:CZ	3:D:1724:PRO:HD2	2.40	0.49
3:D:1467:ILE:HD13	3:D:1763:VAL:HG11	1.94	0.49
3:D:889:LEU:HD11	3:D:975:VAL:HG22	1.95	0.48
3:D:1765:MET:O	3:D:1769:VAL:HG23	2.13	0.48
2:C:56:TYR:CE2	2:C:134:ASP:HB2	2.48	0.48
3:D:167:PHE:CE2	3:D:171:ILE:HD11	2.49	0.48
2:C:134:ASP:OD1	2:C:136:HIS:N	2.31	0.48
3:D:1543:MET:HE1	3:D:1631:ILE:HG21	1.94	0.48
3:D:176:ARG:HB3	3:D:187:ARG:HH22	1.77	0.48
3:D:274:ARG:HD2	3:D:356:GLY:O	2.14	0.48
3:D:276:LYS:HD3	3:D:334:PRO:HB2	1.96	0.48
3:D:1392:ARG:HE	3:D:1724:PRO:HD2	1.72	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:233:LEU:HG	3:D:888:VAL:HG22	1.96	0.48
3:D:749:VAL:O	3:D:753:VAL:HG22	2.13	0.48
3:D:878:SER:HB3	3:D:982:LEU:HD21	1.96	0.47
3:D:833:SER:O	3:D:837:MET:HG2	2.14	0.47
3:D:141:ASN:HD21	3:D:222:ARG:HD3	1.80	0.47
3:D:141:ASN:O	3:D:145:MET:HG3	2.14	0.47
3:D:802:ILE:O	3:D:806:GLU:HG2	2.14	0.47
3:D:1594:PHE:CZ	3:D:1598:ILE:HD11	2.50	0.47
3:D:816:PRO:HA	3:D:818:TYR:H	1.79	0.47
3:D:1564:VAL:O	3:D:1568:LEU:HG	2.14	0.47
7:D:2013:9Z9:C02	7:D:2013:9Z9:C04	2.54	0.47
1:B:152:ARG:HH12	1:B:157:ILE:HG12	1.79	0.47
1:B:168:VAL:O	1:B:172:ILE:HG12	2.14	0.47
3:D:358:ASN:HD22	3:D:362:GLY:HA2	1.79	0.47
1:B:26:SER:HB3	1:B:142:ILE:HG12	1.95	0.47
1:B:56:GLU:OE1	1:B:69:LYS:HD2	2.15	0.47
2:C:68:THR:HB	2:C:77:GLU:OE2	2.15	0.47
3:D:756:ILE:HG22	3:D:757:VAL:HG22	1.96	0.47
3:D:1209:GLU:O	3:D:1213:VAL:HG23	2.15	0.47
3:D:1392:ARG:NH2	3:D:1724:PRO:CD	2.72	0.47
3:D:1392:ARG:NE	3:D:1724:PRO:HD2	2.29	0.47
3:D:751:HIS:HA	3:D:755:LEU:HD13	1.96	0.47
3:D:831:ILE:HA	3:D:834:LEU:HD12	1.97	0.47
3:D:225:LYS:HB3	3:D:225:LYS:HE3	1.71	0.47
3:D:383:ASP:OD2	3:D:944:TRP:N	2.48	0.46
3:D:402:ILE:H	3:D:402:ILE:HD12	1.81	0.46
3:D:874:ILE:HG23	3:D:982:LEU:HD22	1.97	0.46
3:D:786:GLU:O	3:D:787:GLN:HG2	2.15	0.46
3:D:241:ILE:O	3:D:245:LYS:HG2	2.16	0.46
3:D:816:PRO:HA	3:D:818:TYR:N	2.30	0.46
3:D:1471:PHE:HB3	3:D:1475:LYS:NZ	2.31	0.46
1:B:186:ALA:O	1:B:190:GLU:HG2	2.15	0.46
3:D:757:VAL:HG23	3:D:762:VAL:HB	1.97	0.46
3:D:1454:PHE:HA	3:D:1458:PHE:HD2	1.80	0.46
3:D:1252:ILE:O	3:D:1256:LEU:HD23	2.16	0.46
3:D:1712:ASP:OD1	3:D:1713:GLY:N	2.46	0.46
3:D:212:VAL:HG13	3:D:214:ALA:H	1.80	0.46
3:D:390:GLN:HA	3:D:1690:PHE:CZ	2.50	0.46
3:D:963:VAL:O	3:D:967:VAL:HG23	2.16	0.46
3:D:1686:ILE:HG23	3:D:1691:ASN:HB3	1.98	0.46
2:C:79:MET:SD	2:C:80:PHE:N	2.89	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1571:GLY:HA2	3:D:1574:VAL:HG22	1.97	0.46
3:D:146:THR:HG23	3:D:929:PHE:CD2	2.52	0.45
3:D:1430:ARG:HH11	3:D:1437:VAL:HG23	1.82	0.45
3:D:393:LEU:HB2	3:D:1690:PHE:HZ	1.82	0.45
3:D:845:GLU:HG2	3:D:846:GLY:HA2	1.97	0.45
2:C:113:MET:HE3	2:C:114:LEU:N	2.31	0.45
3:D:1516:GLN:HA	3:D:1519:VAL:HB	1.97	0.45
3:D:926:MET:HG2	3:D:935:ILE:HD12	1.99	0.45
3:D:1248:THR:HG21	3:D:1287:LEU:HD12	1.98	0.45
3:D:1360:LYS:HG2	3:D:1431:ASP:C	2.37	0.45
1:B:60:ARG:HB3	1:B:66:GLU:O	2.17	0.45
2:C:61:LYS:HG3	2:C:62:GLN:HG3	1.98	0.45
3:D:770:ILE:HG12	3:D:803:PHE:HZ	1.80	0.45
3:D:1387:LEU:HA	3:D:1387:LEU:HD23	1.83	0.45
2:C:68:THR:OG1	2:C:126:ASN:HB2	2.17	0.45
3:D:184:THR:O	3:D:187:ARG:NH1	2.49	0.45
3:D:273:LEU:HD12	3:D:359:PRO:HG2	1.98	0.45
3:D:1312:LEU:HD22	3:D:1315:LEU:HD11	1.99	0.45
3:D:1474:GLN:HG2	3:D:1478:PHE:CE2	2.52	0.44
3:D:162:THR:O	3:D:166:THR:HG23	2.16	0.44
3:D:236:ILE:HG13	3:D:884:ASN:HB3	1.98	0.44
3:D:1430:ARG:HD3	3:D:1437:VAL:HG23	1.98	0.44
3:D:1516:GLN:HG2	3:D:1578:VAL:HG12	1.98	0.44
7:D:2013:9Z9:C08	7:D:2013:9Z9:C13	2.45	0.44
7:D:2013:9Z9:C09	7:D:2013:9Z9:C12	2.95	0.44
3:D:1315:LEU:HD23	3:D:1321:MET:SD	2.58	0.44
3:D:1696:GLY:O	3:D:1700:ILE:HG23	2.18	0.44
3:D:1715:LEU:HD13	3:D:1751:PHE:CD2	2.52	0.44
2:C:56:TYR:CG	2:C:133:PRO:HD2	2.53	0.44
3:D:414:TYR:OH	3:D:1644:LEU:O	2.36	0.44
1:B:22:VAL:O	1:B:41:ILE:HG21	2.17	0.44
3:D:882:LEU:HD22	3:D:885:LEU:HD12	2.00	0.44
3:D:1514:LYS:HG2	3:D:1515:PHE:H	1.83	0.44
2:C:67:TRP:HZ3	2:C:125:TYR:HB3	1.83	0.44
3:D:1727:ASP:HB3	3:D:1730:THR:HB	2.00	0.44
3:D:859:PHE:CD1	3:D:872:ILE:HD11	2.52	0.44
3:D:1635:ILE:HA	3:D:1638:ALA:HB3	2.00	0.44
3:D:908:TYR:O	3:D:912:VAL:HB	2.18	0.43
3:D:278:LEU:HD21	3:D:318:TYR:HE2	1.82	0.43
3:D:367:ASP:HB2	3:D:1548:ASP:HB3	2.01	0.43
3:D:1303:LEU:HA	3:D:1306:LEU:HD23	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1562:ASN:OD1	3:D:1627:ARG:NH2	2.51	0.43
3:D:1395:ASN:OD1	3:D:1396:VAL:N	2.45	0.43
3:D:1539:ASN:HA	3:D:1542:THR:HG22	2.00	0.43
1:B:28:THR:O	1:B:144:ILE:HA	2.19	0.43
1:B:75:ASN:HB3	1:B:99:LYS:NZ	2.34	0.43
1:B:114:ASN:OD1	6:B:303:NAG:N2	2.51	0.43
3:D:744:ASP:O	3:D:748:LYS:HG2	2.19	0.43
3:D:1339:LEU:O	3:D:1343:LEU:HG	2.18	0.43
1:B:170:LEU:HD13	3:D:1250:ILE:HD11	2.01	0.43
2:C:45:ASP:HB3	2:C:113:MET:CE	2.49	0.43
2:C:56:TYR:HE2	2:C:134:ASP:HB2	1.84	0.43
3:D:270:MET:O	3:D:1621:ARG:NH2	2.52	0.43
3:D:845:GLU:HA	3:D:846:GLY:HA2	1.70	0.43
3:D:1697:ASN:O	3:D:1700:ILE:HG12	2.18	0.43
7:D:2003:9Z9:C11	7:D:2003:9Z9:C07	2.56	0.43
2:C:40:VAL:HG11	2:C:46:ALA:HB2	2.00	0.43
3:D:266:LEU:O	3:D:270:MET:HB2	2.18	0.43
3:D:1496:MET:SD	3:D:1650:MET:HA	2.59	0.43
2:C:79:MET:HE3	2:C:90:LEU:HD11	2.01	0.43
3:D:200:MET:HB3	3:D:218:PHE:HB3	1.99	0.42
3:D:1419:TRP:CE3	3:D:1423:MET:SD	3.12	0.42
3:D:249:ASP:OD1	3:D:249:ASP:N	2.52	0.42
3:D:278:LEU:HD21	3:D:318:TYR:CE2	2.53	0.42
3:D:1593:ASP:HA	3:D:1596:VAL:HG12	2.00	0.42
3:D:1639:LYS:HD2	3:D:1640:GLY:H	1.83	0.42
2:C:96:GLN:HB3	2:C:98:ARG:HE	1.84	0.42
2:C:73:ASN:OD1	2:C:74:ASN:N	2.52	0.42
3:D:1530:ILE:O	3:D:1534:ILE:HG12	2.20	0.42
3:D:1649:MET:HA	3:D:1652:LEU:HG	2.01	0.42
3:D:923:ARG:HD2	3:D:1424:TYR:CE1	2.54	0.42
2:C:100:GLU:HB3	2:C:113:MET:HB3	2.02	0.42
3:D:819:TYR:CZ	3:D:825:ASN:HB3	2.55	0.42
3:D:1469:ASP:O	3:D:1473:GLN:HG2	2.18	0.42
3:D:1252:ILE:HD11	3:D:1284:LEU:HD13	2.02	0.42
3:D:1463:PHE:CE2	3:D:1467:ILE:HD11	2.55	0.42
3:D:1543:MET:HG2	3:D:1627:ARG:CZ	2.50	0.42
3:D:1687:ASP:OD1	3:D:1687:ASP:N	2.53	0.42
3:D:149:ASN:OD1	3:D:149:ASN:N	2.53	0.42
3:D:173:ILE:HG13	3:D:185:PHE:HE1	1.85	0.42
3:D:199:VAL:O	3:D:203:VAL:HG23	2.19	0.42
3:D:425:MET:HE2	3:D:1774:PHE:HA	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1321:MET:SD	3:D:1664:LEU:HD22	2.59	0.42
3:D:432:GLN:O	3:D:436:GLU:HG2	2.20	0.42
3:D:913:CYS:HB2	3:D:919:CYS:HB3	1.95	0.42
2:C:50:CYS:HB2	2:C:67:TRP:CZ2	2.55	0.41
3:D:261:PHE:HB3	3:D:376:LEU:CD2	2.50	0.41
3:D:1412:GLN:HG2	3:D:1711:TRP:CZ2	2.55	0.41
1:B:28:THR:OG1	1:B:29:GLU:OE1	2.35	0.41
3:D:1345:PHE:HE2	3:D:1454:PHE:HB3	1.85	0.41
3:D:376:LEU:HG	3:D:379:LEU:HD12	2.03	0.41
3:D:1463:PHE:O	3:D:1466:VAL:HG12	2.20	0.41
3:D:753:VAL:O	3:D:756:ILE:HD12	2.20	0.41
2:C:93:GLU:H	2:C:93:GLU:CD	2.24	0.41
3:D:407:VAL:O	3:D:411:GLY:N	2.49	0.41
3:D:877:ASN:OD1	3:D:881:ALA:HB3	2.21	0.41
3:D:1309:LEU:HD12	3:D:1312:LEU:HD12	2.02	0.41
3:D:1486:THR:O	3:D:1490:LYS:HG3	2.21	0.41
3:D:250:VAL:HG21	3:D:422:VAL:HG11	2.03	0.41
3:D:968:MET:O	3:D:972:ASN:HB2	2.21	0.41
3:D:134:ILE:HA	3:D:137:THR:HG22	2.03	0.41
3:D:237:VAL:O	3:D:241:ILE:HG12	2.20	0.41
3:D:264:ILE:HG12	3:D:1628:ILE:HG13	2.03	0.41
3:D:366:PHE:HE2	3:D:376:LEU:HD11	1.85	0.41
3:D:751:HIS:ND1	3:D:755:LEU:HD22	2.36	0.41
3:D:912:VAL:HG21	3:D:921:LEU:HA	2.02	0.41
3:D:1222:ALA:HB1	3:D:1240:LEU:HD22	2.01	0.41
3:D:1396:VAL:O	3:D:1397:LYS:HB2	2.21	0.41
1:B:36:PHE:HB2	1:B:111:VAL:HG21	2.02	0.41
3:D:804:THR:CG2	3:D:836:LEU:HD21	2.51	0.41
3:D:923:ARG:NH2	3:D:1428:ASP:OD2	2.54	0.41
3:D:925:HIS:O	3:D:931:HIS:HB3	2.20	0.41
3:D:1395:ASN:HD21	3:D:1399:ASN:HD21	1.67	0.41
2:C:129:ILE:O	2:C:137:ARG:HA	2.21	0.40
3:D:1627:ARG:HG2	3:D:1630:ARG:HH22	1.86	0.40
3:D:119:LYS:O	3:D:122:ILE:HG22	2.21	0.40
3:D:1554:MET:O	3:D:1558:LEU:HD23	2.22	0.40
1:B:56:GLU:HB2	1:B:122:HIS:HB2	2.02	0.40
3:D:239:ALA:HA	3:D:242:GLN:HG2	2.03	0.40
3:D:421:ALA:O	3:D:425:MET:HG3	2.22	0.40
3:D:913:CYS:HA	3:D:919:CYS:HA	2.04	0.40
1:B:20:GLY:N	3:D:1693:GLU:OE2	2.54	0.40
1:B:57:TRP:HB2	1:B:71:LEU:HG	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:923:ARG:HH22	3:D:1428:ASP:CG	2.25	0.40
3:D:1215:MET:SD	3:D:1250:ILE:HG21	2.61	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	B	171/218 (78%)	160 (94%)	11 (6%)	0	100	100
2	C	124/215 (58%)	113 (91%)	11 (9%)	0	100	100
3	D	1119/1951 (57%)	1042 (93%)	77 (7%)	0	100	100
All	All	1414/2384 (59%)	1315 (93%)	99 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	157/190 (83%)	157 (100%)	0	100	100
2	C	118/193 (61%)	118 (100%)	0	100	100
3	D	998/1725 (58%)	995 (100%)	3 (0%)	91	94
All	All	1273/2108 (60%)	1270 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1384	CYS
3	D	1389	LYS
3	D	1390	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
3	D	141	ASN
3	D	358	ASN
3	D	1390	GLN
3	D	1470	ASN
3	D	1516	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	E	1	3,4	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	BMA	E	3	4	11,11,12	0.89	1 (9%)	15,15,17	1.16	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	1	3,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	F	2	5	14,14,15	0.44	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	BMA	C1-C2	2.04	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	O2-C2-C3	-2.63	104.86	110.14
4	E	3	BMA	C1-C2-C3	-2.27	106.88	109.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

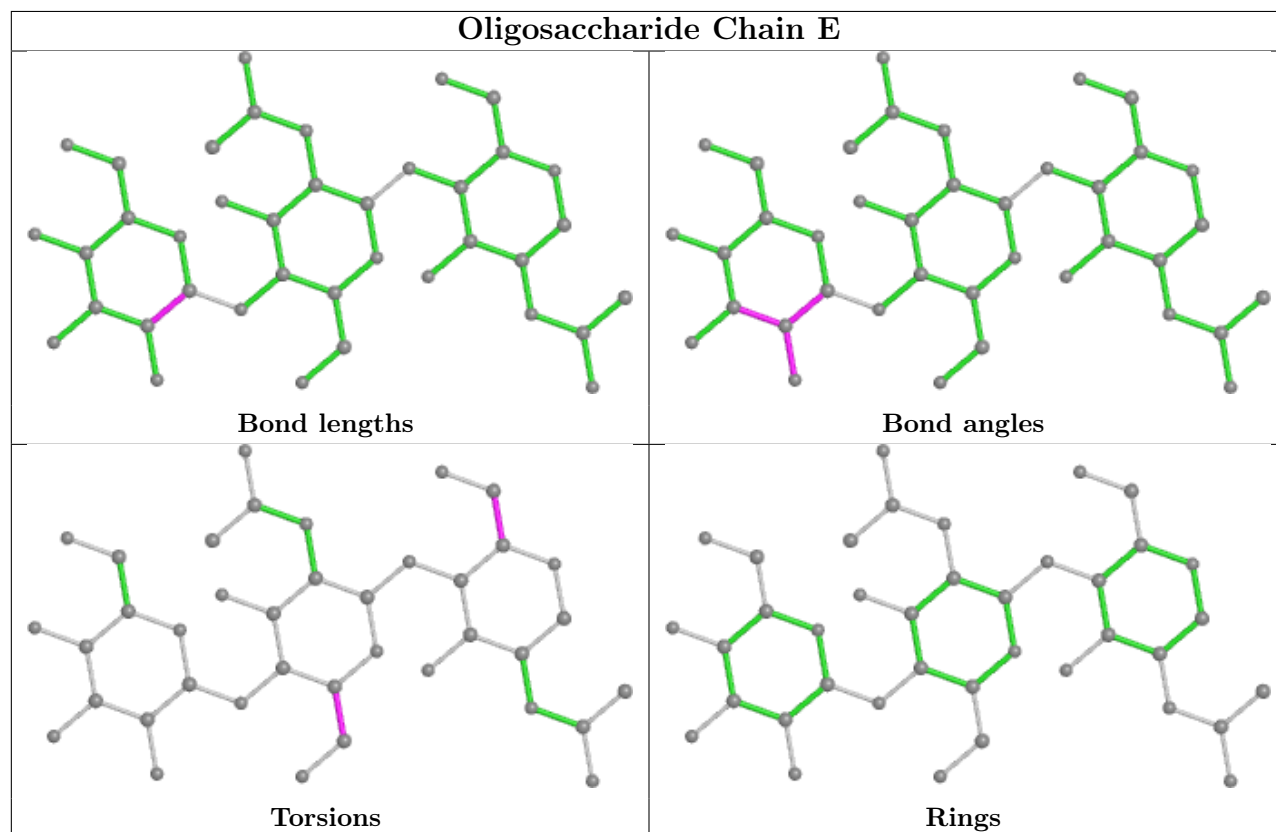
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7

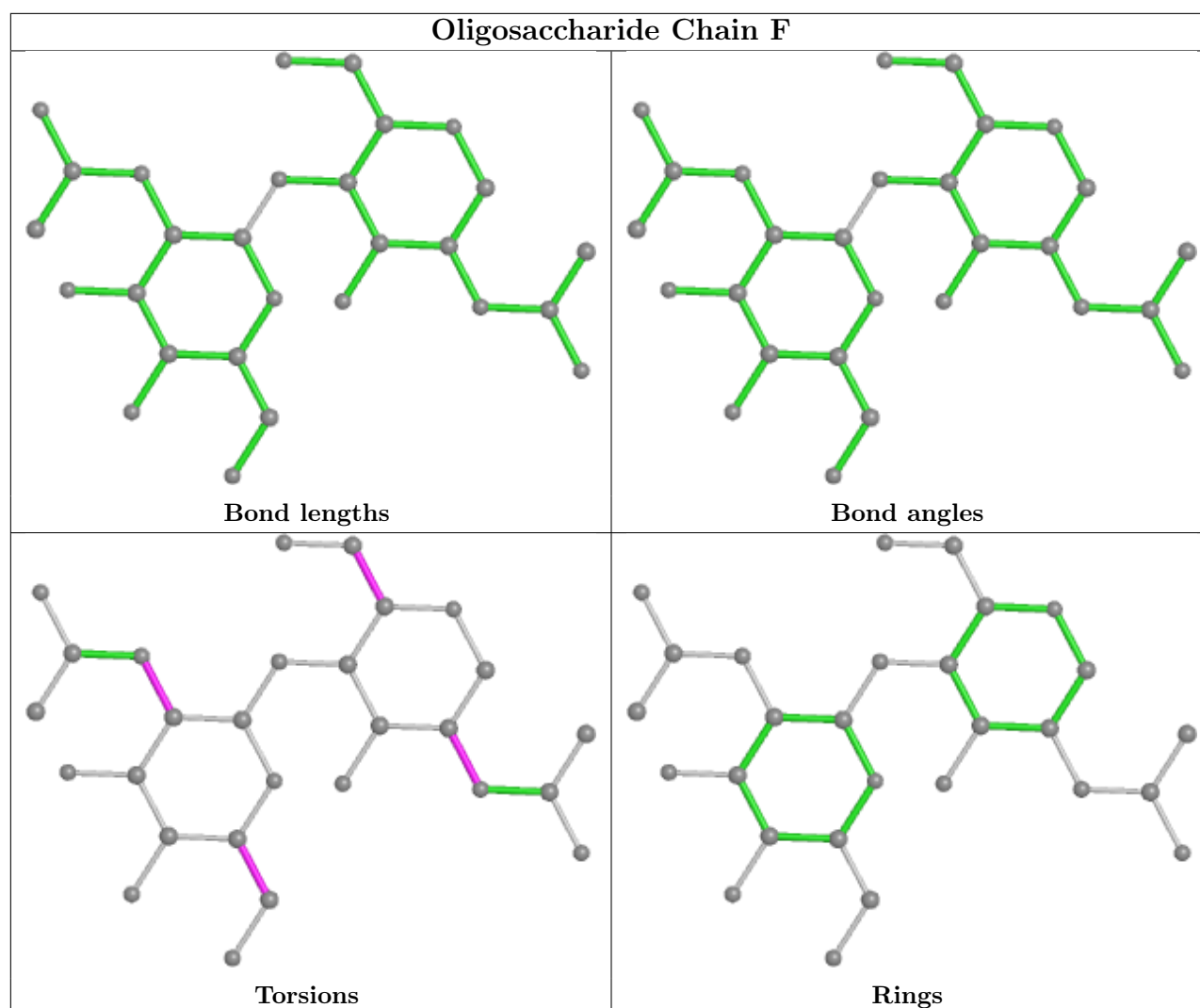


There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

25 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	$\# Z  > 2$
6	NAG	B	303	1	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
8	6OU	D	2006	-	27,27,48	1.02	4 (14%)	29,29,53	1.25	2 (6%)
6	NAG	B	302	1	14,14,15	0.19	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	6OU	D	2007	-	32,32,48	1.07	4 (12%)	35,37,53	1.14	2 (5%)
8	6OU	D	2016	-	12,12,48	1.02	2 (16%)	12,12,53	1.07	1 (8%)
8	6OU	D	2019	-	12,12,48	1.02	2 (16%)	12,12,53	1.05	0
7	9Z9	D	2003	-	37,37,44	10.79	29 (78%)	60,60,68	2.08	17 (28%)
6	NAG	D	2001	3	14,14,15	0.26	0	17,19,21	0.46	0
8	6OU	D	2011	-	13,13,48	0.99	2 (15%)	13,13,53	1.06	1 (7%)
8	6OU	D	2017	-	12,12,48	1.03	2 (16%)	12,12,53	1.07	1 (8%)
8	6OU	D	2012	-	10,10,48	0.31	0	9,9,53	0.75	0
8	6OU	D	2010	-	13,13,48	0.98	2 (15%)	13,13,53	1.02	0
8	6OU	D	2008	-	36,36,48	1.01	4 (11%)	39,41,53	1.14	2 (5%)
7	9Z9	D	2013	-	37,37,44	10.78	29 (78%)	60,60,68	2.11	20 (33%)
8	6OU	D	2015	-	12,12,48	1.03	2 (16%)	12,12,53	0.99	0
9	966	D	2021	-	50,51,51	1.89	6 (12%)	67,83,83	1.91	14 (20%)
6	NAG	B	304	1	14,14,15	0.26	0	17,19,21	0.36	0
8	6OU	D	2004	-	8,8,48	0.29	0	7,7,53	0.77	0
8	6OU	D	2005	-	36,36,48	1.06	5 (13%)	40,41,53	1.16	2 (5%)
8	6OU	D	2018	-	12,12,48	1.03	2 (16%)	12,12,53	1.05	1 (8%)
8	6OU	D	2009	-	26,26,48	1.20	4 (15%)	28,28,53	1.41	3 (10%)
8	6OU	D	2014	-	12,12,48	1.03	2 (16%)	12,12,53	1.04	0
6	NAG	B	301	1	14,14,15	0.23	0	17,19,21	0.42	0
7	9Z9	D	2002	-	37,37,44	10.81	29 (78%)	60,60,68	1.91	19 (31%)
8	6OU	D	2020	-	10,10,48	0.33	0	9,9,53	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
6	NAG	B	303	1	-	0/6/23/26	0/1/1/1
8	6OU	D	2006	-	-	12/29/29/52	-
6	NAG	B	302	1	-	1/6/23/26	0/1/1/1
8	6OU	D	2007	-	-	12/36/36/52	-
8	6OU	D	2016	-	-	3/11/11/52	-
8	6OU	D	2019	-	-	2/11/11/52	-
7	9Z9	D	2003	-	-	0/3/91/100	0/6/6/6
6	NAG	D	2001	3	-	2/6/23/26	0/1/1/1
8	6OU	D	2011	-	-	7/12/12/52	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6OU	D	2017	-	-	1/11/11/52	-
8	6OU	D	2012	-	-	2/8/8/52	-
8	6OU	D	2010	-	-	4/12/12/52	-
8	6OU	D	2008	-	-	16/40/40/52	-
7	9Z9	D	2013	-	-	3/3/91/100	0/6/6/6
8	6OU	D	2015	-	-	6/11/11/52	-
9	966	D	2021	-	-	12/27/126/126	0/1/7/7
6	NAG	B	304	1	-	0/6/23/26	0/1/1/1
8	6OU	D	2004	-	-	0/6/6/52	-
8	6OU	D	2005	-	-	12/38/38/52	-
8	6OU	D	2018	-	-	9/11/11/52	-
8	6OU	D	2009	-	-	14/27/27/52	-
8	6OU	D	2014	-	-	3/11/11/52	-
6	NAG	B	301	1	-	2/6/23/26	0/1/1/1
7	9Z9	D	2002	-	-	2/3/91/100	0/6/6/6
8	6OU	D	2020	-	-	3/7/8/52	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2002	9Z9	C76-C73	-26.20	1.10	1.52
7	D	2003	9Z9	C76-C73	-26.03	1.10	1.52
7	D	2013	9Z9	C76-C73	-25.99	1.10	1.52
7	D	2002	9Z9	C15-C07	-21.46	1.16	1.53
7	D	2003	9Z9	C15-C07	-21.33	1.17	1.53
7	D	2013	9Z9	C15-C07	-21.01	1.17	1.53
7	D	2002	9Z9	C07-C06	-20.27	1.14	1.53
7	D	2003	9Z9	C07-C06	-20.10	1.15	1.53
7	D	2002	9Z9	O72-C73	-20.07	0.98	1.42
7	D	2003	9Z9	O72-C73	-19.98	0.98	1.42
7	D	2013	9Z9	C07-C06	-19.97	1.15	1.53
7	D	2013	9Z9	O72-C73	-19.92	0.98	1.42
7	D	2013	9Z9	C11-C13	-18.14	1.16	1.52
7	D	2003	9Z9	C11-C13	-17.74	1.17	1.52
7	D	2002	9Z9	C11-C13	-17.55	1.18	1.52
7	D	2013	9Z9	C10-C02	-16.55	1.24	1.54
7	D	2003	9Z9	C10-C02	-16.45	1.24	1.54
7	D	2002	9Z9	C10-C02	-16.38	1.24	1.54
7	D	2003	9Z9	C79-C78	-15.41	1.13	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2013	9Z9	C79-C78	-15.39	1.13	1.51
7	D	2002	9Z9	C79-C78	-15.24	1.14	1.51
7	D	2013	9Z9	C05-C04	13.77	1.83	1.52
7	D	2003	9Z9	C05-C04	13.56	1.82	1.52
7	D	2002	9Z9	C05-C04	13.44	1.82	1.52
7	D	2013	9Z9	C81-C78	12.17	1.91	1.52
7	D	2002	9Z9	C81-C78	12.15	1.91	1.52
7	D	2003	9Z9	C81-C78	12.14	1.91	1.52
7	D	2002	9Z9	C11-C08	12.12	1.76	1.56
7	D	2003	9Z9	C11-C08	11.96	1.76	1.56
7	D	2013	9Z9	C03-C74	-11.66	1.16	1.54
7	D	2003	9Z9	C03-C74	-11.64	1.16	1.54
7	D	2002	9Z9	C03-C74	-11.51	1.16	1.54
7	D	2013	9Z9	C11-C08	11.49	1.75	1.56
7	D	2013	9Z9	C10-C09	-11.43	1.29	1.53
7	D	2003	9Z9	C10-C09	-11.20	1.29	1.53
7	D	2002	9Z9	C10-C09	-11.16	1.29	1.53
7	D	2002	9Z9	C02-C03	10.29	1.77	1.56
7	D	2003	9Z9	C02-C03	10.20	1.76	1.56
7	D	2002	9Z9	C73-C74	10.14	1.73	1.53
7	D	2013	9Z9	C73-C74	10.00	1.73	1.53
7	D	2003	9Z9	C73-C74	9.96	1.73	1.53
7	D	2013	9Z9	C02-C03	9.94	1.76	1.56
7	D	2002	9Z9	C19-C11	9.80	1.72	1.54
7	D	2003	9Z9	C19-C11	9.74	1.72	1.54
7	D	2013	9Z9	C19-C11	9.69	1.72	1.54
7	D	2002	9Z9	C07-C08	-9.67	1.35	1.53
7	D	2003	9Z9	C07-C08	-9.59	1.35	1.53
7	D	2013	9Z9	C07-C08	-9.46	1.35	1.53
7	D	2013	9Z9	C77-C78	-8.41	1.29	1.52
7	D	2003	9Z9	C77-C78	-8.38	1.29	1.52
7	D	2002	9Z9	C77-C78	-8.23	1.29	1.52
7	D	2013	9Z9	C03-C04	-8.02	1.38	1.54
7	D	2002	9Z9	C03-C04	-7.98	1.38	1.54
7	D	2003	9Z9	C03-C04	-7.96	1.38	1.54
9	D	2021	966	C01-C02	7.75	1.69	1.56
7	D	2002	9Z9	C18-C17	-7.75	1.30	1.51
7	D	2013	9Z9	C18-C17	-7.67	1.30	1.51
7	D	2003	9Z9	C18-C17	-7.65	1.30	1.51
7	D	2002	9Z9	O80-C73	-7.58	1.30	1.42
7	D	2003	9Z9	O80-C73	-7.31	1.31	1.42
7	D	2013	9Z9	O80-C73	-7.22	1.31	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2013	9Z9	C15-C14	6.44	1.64	1.50
7	D	2003	9Z9	C15-C14	6.26	1.63	1.50
9	D	2021	966	C01-C03	6.23	1.65	1.56
7	D	2002	9Z9	C15-C14	6.10	1.63	1.50
7	D	2002	9Z9	C75-C74	5.34	1.65	1.53
7	D	2013	9Z9	C75-C74	5.28	1.64	1.53
7	D	2003	9Z9	C75-C74	5.27	1.64	1.53
7	D	2003	9Z9	O72-C04	5.02	1.54	1.43
7	D	2013	9Z9	O72-C04	4.97	1.54	1.43
7	D	2003	9Z9	C16-C13	4.95	1.62	1.51
7	D	2013	9Z9	C16-C13	4.92	1.62	1.51
7	D	2002	9Z9	C16-C13	4.88	1.62	1.51
7	D	2002	9Z9	O72-C04	4.81	1.54	1.43
9	D	2021	966	C03-C08	4.26	1.64	1.53
9	D	2021	966	C07-C06	4.00	1.58	1.54
8	D	2009	6OU	O30-C20	-3.87	1.40	1.47
7	D	2013	9Z9	O20-C17	3.62	1.53	1.43
7	D	2003	9Z9	O20-C17	3.51	1.53	1.43
7	D	2002	9Z9	O20-C17	3.48	1.53	1.43
7	D	2013	9Z9	C16-C17	3.48	1.60	1.52
7	D	2013	9Z9	C09-C08	-3.45	1.48	1.53
7	D	2003	9Z9	C16-C17	3.41	1.60	1.52
9	D	2021	966	C06-C02	3.39	1.61	1.55
7	D	2002	9Z9	C16-C17	3.24	1.59	1.52
7	D	2002	9Z9	O80-C79	3.18	1.48	1.43
7	D	2013	9Z9	O80-C79	3.09	1.48	1.43
7	D	2003	9Z9	O80-C79	3.09	1.48	1.43
7	D	2002	9Z9	C09-C08	-3.07	1.48	1.53
7	D	2003	9Z9	C09-C08	-3.07	1.48	1.53
7	D	2013	9Z9	C05-C06	3.02	1.60	1.54
9	D	2021	966	C05-C04	2.94	1.59	1.54
7	D	2003	9Z9	C05-C06	2.88	1.60	1.54
7	D	2002	9Z9	C05-C06	2.79	1.60	1.54
8	D	2005	6OU	P23-O26	2.69	1.65	1.54
8	D	2007	6OU	O18-C16	2.52	1.40	1.33
8	D	2007	6OU	O30-C20	-2.51	1.40	1.46
8	D	2008	6OU	O30-C20	-2.51	1.40	1.46
8	D	2005	6OU	O30-C20	-2.48	1.40	1.46
8	D	2006	6OU	O30-C20	-2.47	1.40	1.46
8	D	2008	6OU	O18-C16	2.42	1.40	1.33
8	D	2009	6OU	O18-C16	2.42	1.40	1.33
8	D	2005	6OU	O18-C16	2.39	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	6OU	O18-C16	2.37	1.40	1.33
8	D	2019	6OU	O18-C16	2.34	1.40	1.33
8	D	2014	6OU	O18-C16	2.33	1.40	1.33
8	D	2016	6OU	O18-C16	2.32	1.40	1.33
8	D	2011	6OU	O18-C16	2.32	1.40	1.33
8	D	2018	6OU	O18-C16	2.31	1.40	1.33
8	D	2017	6OU	O18-C16	2.31	1.40	1.33
8	D	2015	6OU	O18-C16	2.30	1.40	1.33
8	D	2010	6OU	O18-C16	2.29	1.40	1.33
8	D	2006	6OU	O30-C31	2.16	1.40	1.34
8	D	2009	6OU	O30-C31	2.16	1.40	1.34
8	D	2005	6OU	O30-C31	2.16	1.40	1.34
8	D	2007	6OU	O30-C31	2.15	1.40	1.34
8	D	2018	6OU	O18-C19	-2.14	1.40	1.45
8	D	2011	6OU	O18-C19	-2.14	1.40	1.45
8	D	2008	6OU	O30-C31	2.13	1.40	1.34
8	D	2008	6OU	O18-C19	-2.12	1.40	1.45
8	D	2010	6OU	O18-C19	-2.12	1.40	1.45
8	D	2005	6OU	O18-C19	-2.12	1.40	1.45
8	D	2015	6OU	O18-C19	-2.12	1.40	1.45
8	D	2009	6OU	O18-C19	-2.11	1.40	1.45
8	D	2006	6OU	O18-C19	-2.10	1.40	1.45
8	D	2014	6OU	O18-C19	-2.10	1.40	1.45
8	D	2016	6OU	O18-C19	-2.10	1.40	1.45
8	D	2017	6OU	O18-C19	-2.09	1.40	1.45
8	D	2019	6OU	O18-C19	-2.08	1.40	1.45
8	D	2007	6OU	O18-C19	-2.08	1.40	1.45

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	2021	966	C05-C08-C03	-7.23	99.67	104.80
9	D	2021	966	C01-C04-N01	6.15	119.31	110.70
7	D	2003	9Z9	O80-C73-C76	5.73	116.10	110.77
7	D	2013	9Z9	O80-C73-C76	5.71	116.08	110.77
7	D	2013	9Z9	C10-C02-C06	5.57	115.92	107.27
7	D	2003	9Z9	C10-C02-C06	4.53	114.30	107.27
7	D	2013	9Z9	C76-C73-C74	-4.38	106.68	115.69
7	D	2003	9Z9	C76-C73-C74	-4.37	106.71	115.69
7	D	2002	9Z9	C10-C02-C06	4.32	113.98	107.27
7	D	2002	9Z9	C08-C11-C13	4.14	116.14	109.65
9	D	2021	966	C01-C02-C06	4.10	121.79	117.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2003	9Z9	C08-C11-C13	4.09	116.06	109.65
8	D	2005	6OU	O30-C31-C33	4.02	120.16	111.50
8	D	2007	6OU	O30-C31-C33	3.95	120.02	111.50
8	D	2009	6OU	O30-C31-C33	3.93	119.97	111.50
8	D	2008	6OU	O30-C31-C33	3.90	119.91	111.50
8	D	2006	6OU	O30-C31-C33	3.89	119.88	111.50
7	D	2013	9Z9	C15-C14-C13	-3.89	117.89	125.06
7	D	2003	9Z9	C12-C11-C08	-3.85	107.09	111.68
7	D	2002	9Z9	C76-C73-C74	-3.70	108.09	115.69
7	D	2002	9Z9	C10-C02-C03	3.68	121.33	115.46
7	D	2013	9Z9	C01-C02-C10	-3.64	104.85	110.59
7	D	2003	9Z9	C01-C02-C10	-3.64	104.85	110.59
7	D	2002	9Z9	C12-C11-C08	-3.54	107.46	111.68
9	D	2021	966	C12-C11-C16	-3.52	105.22	110.73
7	D	2013	9Z9	C10-C02-C03	3.50	121.06	115.46
7	D	2003	9Z9	C10-C02-C03	3.43	120.94	115.46
7	D	2013	9Z9	C05-C06-C07	3.41	126.77	119.48
7	D	2002	9Z9	C15-C14-C13	-3.39	118.81	125.06
7	D	2003	9Z9	C15-C14-C13	-3.34	118.90	125.06
7	D	2003	9Z9	C02-C03-C04	3.32	108.15	104.13
7	D	2002	9Z9	C01-C02-C10	-3.31	105.37	110.59
7	D	2013	9Z9	C11-C13-C14	-3.23	117.96	122.90
7	D	2002	9Z9	O80-C73-C76	3.19	113.74	110.77
9	D	2021	966	C07-C05-C04	-3.17	106.02	111.14
7	D	2013	9Z9	C12-C11-C08	-3.17	107.90	111.68
7	D	2002	9Z9	C01-C02-C03	-3.14	104.00	111.63
9	D	2021	966	C05-C04-N01	-3.13	112.64	115.63
7	D	2013	9Z9	C15-C07-C08	3.01	113.36	109.71
8	D	2009	6OU	C20-O30-C31	-3.00	114.02	117.88
7	D	2003	9Z9	C01-C02-C03	-2.99	104.36	111.63
7	D	2013	9Z9	C05-C06-C02	-2.93	100.00	103.91
7	D	2003	9Z9	C05-C06-C07	2.92	125.73	119.48
7	D	2002	9Z9	C02-C03-C04	2.78	107.50	104.13
9	D	2021	966	C15-C09-C03	2.76	110.42	108.20
7	D	2013	9Z9	C01-C02-C03	-2.76	104.90	111.63
9	D	2021	966	C15-N01-C04	2.76	121.09	115.46
7	D	2013	9Z9	C75-C74-C73	-2.72	109.95	114.92
8	D	2009	6OU	O18-C16-C15	2.72	120.43	111.91
9	D	2021	966	C03-C01-C04	-2.69	92.94	99.01
9	D	2021	966	O01-C22-O08	2.66	128.50	123.61
9	D	2021	966	C17-C18-C10	2.66	115.74	110.63
9	D	2021	966	C17-C09-C03	-2.65	106.76	110.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2003	9Z9	C03-C02-C06	2.64	104.12	100.23
7	D	2002	9Z9	C75-C74-C73	-2.64	110.10	114.92
8	D	2008	6OU	O18-C16-C15	2.64	120.18	111.91
7	D	2013	9Z9	C02-C03-C04	2.60	107.28	104.13
8	D	2005	6OU	O18-C16-C15	2.58	120.01	111.91
8	D	2006	6OU	O18-C16-C15	2.56	119.94	111.91
6	B	303	NAG	C1-O5-C5	2.55	115.65	112.19
9	D	2021	966	O03-C10-C01	2.54	113.05	108.35
7	D	2003	9Z9	C75-C74-C73	-2.52	110.31	114.92
7	D	2003	9Z9	C02-C03-C74	-2.52	111.98	120.56
7	D	2002	9Z9	C08-C07-C06	2.51	112.45	109.09
7	D	2002	9Z9	C03-C02-C06	2.49	103.89	100.23
7	D	2013	9Z9	C09-C08-C11	-2.48	109.82	113.08
7	D	2013	9Z9	C02-C03-C74	-2.46	112.18	120.56
8	D	2007	6OU	O18-C16-C15	2.45	119.58	111.91
7	D	2002	9Z9	C01-C02-C06	-2.44	107.16	111.71
7	D	2002	9Z9	C02-C03-C74	-2.42	112.33	120.56
7	D	2003	9Z9	C01-C02-C06	-2.41	107.21	111.71
7	D	2002	9Z9	C05-C06-C07	2.40	124.62	119.48
7	D	2013	9Z9	C01-C02-C06	-2.40	107.25	111.71
9	D	2021	966	C01-C04-C05	-2.39	96.50	100.89
7	D	2003	9Z9	C05-C06-C02	-2.36	100.76	103.91
7	D	2013	9Z9	C75-C74-C03	-2.27	109.47	114.50
7	D	2002	9Z9	C05-C06-C02	-2.26	100.91	103.91
7	D	2013	9Z9	C16-C13-C11	-2.14	113.58	116.42
7	D	2003	9Z9	C16-C13-C11	-2.11	113.62	116.42
7	D	2002	9Z9	C77-C78-C79	2.10	111.48	108.56
8	D	2017	6OU	O18-C16-C15	2.08	120.46	112.23
7	D	2002	9Z9	C11-C08-C07	-2.07	109.63	112.73
7	D	2013	9Z9	C08-C11-C13	2.04	112.85	109.65
8	D	2011	6OU	O18-C16-C15	2.04	120.28	112.23
8	D	2018	6OU	O18-C16-C15	2.01	120.16	112.23
8	D	2016	6OU	O18-C16-C15	2.00	120.14	112.23

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	2013	9Z9	C16-C17-O20-C21
8	D	2005	6OU	O30-C20-C21-O22
8	D	2007	6OU	C15-C16-O18-C19
8	D	2007	6OU	O17-C16-O18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	D	2007	6OU	C27-O26-P23-O24
8	D	2007	6OU	C27-O26-P23-O25
8	D	2008	6OU	C21-O22-P23-O24
8	D	2008	6OU	C27-O26-P23-O24
8	D	2008	6OU	O26-C27-C28-N29
8	D	2009	6OU	O18-C19-C20-C21
8	D	2009	6OU	O18-C19-C20-O30
8	D	2011	6OU	C15-C16-O18-C19
8	D	2011	6OU	O17-C16-O18-C19
8	D	2019	6OU	C15-C16-O18-C19
8	D	2020	6OU	C13-C14-C15-C16
9	D	2021	966	C18-C10-O03-C26
9	D	2021	966	C24-C20-N01-C15
9	D	2021	966	C24-C20-N01-C04
9	D	2021	966	C15-C09-C19-O06
9	D	2021	966	C17-C09-C19-O06
9	D	2021	966	C03-C09-C19-O06
8	D	2019	6OU	O17-C16-O18-C19
8	D	2008	6OU	O17-C16-O18-C19
8	D	2018	6OU	O17-C16-O18-C19
8	D	2008	6OU	C15-C16-O18-C19
8	D	2018	6OU	C15-C16-O18-C19
6	D	2001	NAG	O5-C5-C6-O6
8	D	2009	6OU	C15-C16-O18-C19
8	D	2009	6OU	O17-C16-O18-C19
6	D	2001	NAG	C4-C5-C6-O6
8	D	2006	6OU	C31-C33-C34-C35
8	D	2008	6OU	C13-C14-C15-C16
8	D	2015	6OU	C15-C16-O18-C19
8	D	2009	6OU	C13-C14-C15-C16
8	D	2011	6OU	C13-C14-C15-C16
8	D	2012	6OU	C02-C03-C04-C05
6	B	302	NAG	O5-C5-C6-O6
8	D	2009	6OU	C31-C33-C34-C35
8	D	2007	6OU	C33-C31-O30-C20
8	D	2007	6OU	C27-O26-P23-O22
8	D	2008	6OU	C27-O26-P23-O22
6	B	301	NAG	C4-C5-C6-O6
8	D	2007	6OU	O32-C31-O30-C20
8	D	2015	6OU	C11-C12-C13-C14
8	D	2005	6OU	C15-C16-O18-C19
8	D	2005	6OU	C33-C31-O30-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	D	2008	6OU	C33-C31-O30-C20
8	D	2005	6OU	O32-C31-O30-C20
8	D	2008	6OU	O32-C31-O30-C20
8	D	2008	6OU	C34-C35-C36-C37
7	D	2002	9Z9	C16-C17-O20-C21
7	D	2002	9Z9	C18-C17-O20-C21
8	D	2005	6OU	O17-C16-O18-C19
8	D	2015	6OU	C09-C10-C11-C12
9	D	2021	966	C32-C34-O09-C35
9	D	2021	966	C33-C34-O09-C35
8	D	2015	6OU	O17-C16-O18-C19
8	D	2009	6OU	O32-C31-O30-C20
8	D	2009	6OU	C33-C31-O30-C20
8	D	2006	6OU	C12-C13-C14-C15
8	D	2008	6OU	C21-O22-P23-O26
8	D	2006	6OU	C07-C08-C09-C10
8	D	2006	6OU	C33-C34-C35-C36
6	B	301	NAG	O5-C5-C6-O6
8	D	2006	6OU	C15-C16-O18-C19
8	D	2014	6OU	C15-C16-O18-C19
8	D	2009	6OU	C21-C20-O30-C31
8	D	2012	6OU	C06-C07-C08-C09
8	D	2006	6OU	O18-C19-C20-O30
9	D	2021	966	C09-C19-O06-C29
8	D	2011	6OU	C10-C11-C12-C13
8	D	2005	6OU	C19-C20-C21-O22
8	D	2007	6OU	C19-C20-C21-O22
8	D	2006	6OU	O17-C16-O18-C19
8	D	2020	6OU	C07-C08-C09-C10
8	D	2018	6OU	C13-C14-C15-C16
8	D	2011	6OU	C06-C07-C08-C09
8	D	2005	6OU	O30-C31-C33-C34
7	D	2013	9Z9	C22-C21-O20-C17
8	D	2005	6OU	C31-C33-C34-C35
8	D	2007	6OU	C31-C33-C34-C35
8	D	2009	6OU	C11-C12-C13-C14
9	D	2021	966	C01-C10-O03-C26
9	D	2021	966	C11-C13-C21-C25
8	D	2010	6OU	C09-C10-C11-C12
9	D	2021	966	C11-C13-C21-O07
7	D	2013	9Z9	C18-C17-O20-C21
8	D	2016	6OU	C08-C09-C10-C11

*Continued on next page...*

*Continued from previous page...*

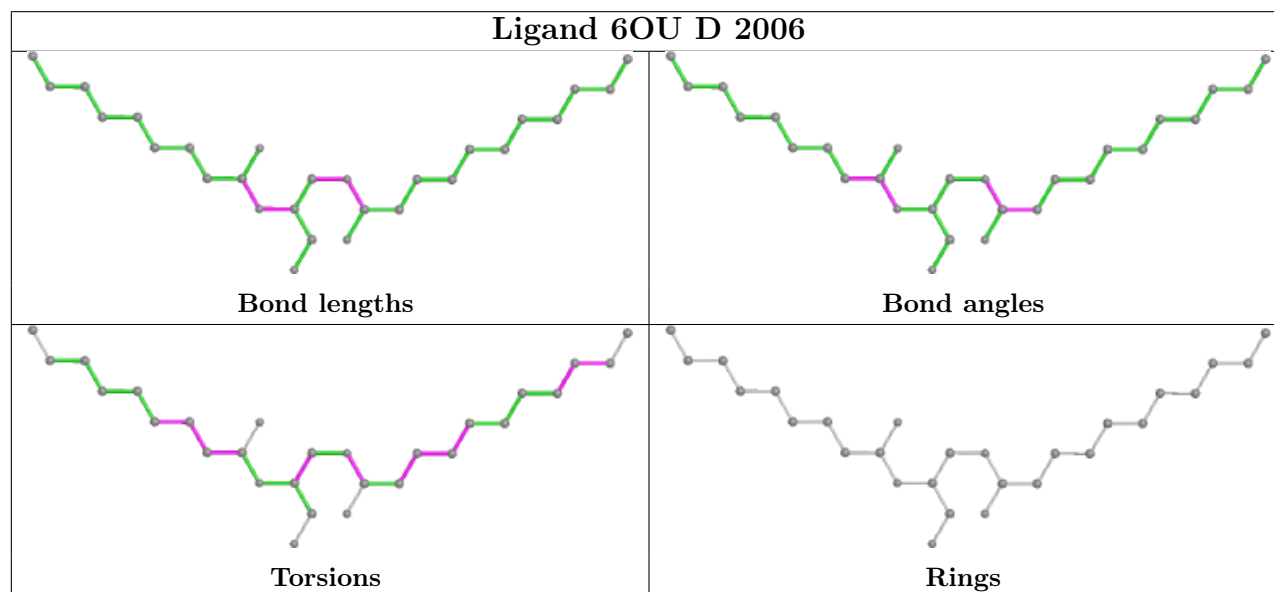
Mol	Chain	Res	Type	Atoms
8	D	2007	6OU	C21-O22-P23-O26
8	D	2011	6OU	C11-C12-C13-C14
8	D	2007	6OU	C38-C39-C40-C41
8	D	2007	6OU	O30-C20-C21-O22
8	D	2018	6OU	C09-C10-C11-C12
8	D	2006	6OU	O18-C19-C20-C21
8	D	2008	6OU	C35-C36-C37-C38
8	D	2006	6OU	C06-C07-C08-C09
8	D	2009	6OU	C06-C07-C08-C09
8	D	2016	6OU	C11-C12-C13-C14
8	D	2014	6OU	O17-C16-O18-C19
8	D	2005	6OU	C38-C39-C40-C41
8	D	2020	6OU	C08-C09-C10-C11
8	D	2010	6OU	C11-C12-C13-C14
8	D	2010	6OU	C08-C09-C10-C11
8	D	2018	6OU	C11-C12-C13-C14
8	D	2006	6OU	C11-C12-C13-C14
8	D	2006	6OU	C13-C14-C15-C16
8	D	2015	6OU	C08-C09-C10-C11
8	D	2014	6OU	C08-C09-C10-C11
8	D	2009	6OU	C19-C20-O30-C31
8	D	2010	6OU	C10-C11-C12-C13
8	D	2016	6OU	C10-C11-C12-C13
8	D	2015	6OU	C14-C15-C16-O18
8	D	2017	6OU	C10-C11-C12-C13
8	D	2018	6OU	C08-C09-C10-C11
8	D	2011	6OU	C08-C09-C10-C11
8	D	2009	6OU	C07-C08-C09-C10
8	D	2018	6OU	C14-C15-C16-O18
8	D	2008	6OU	C14-C15-C16-O18
8	D	2008	6OU	C38-C39-C40-C41
8	D	2008	6OU	C12-C13-C14-C15
8	D	2005	6OU	O32-C31-C33-C34
8	D	2009	6OU	C34-C35-C36-C37
8	D	2005	6OU	C40-C41-C42-C43
8	D	2018	6OU	C12-C13-C14-C15
8	D	2018	6OU	C14-C15-C16-O17
8	D	2008	6OU	C14-C15-C16-O17
8	D	2005	6OU	C14-C15-C16-O18
8	D	2006	6OU	O30-C31-C33-C34

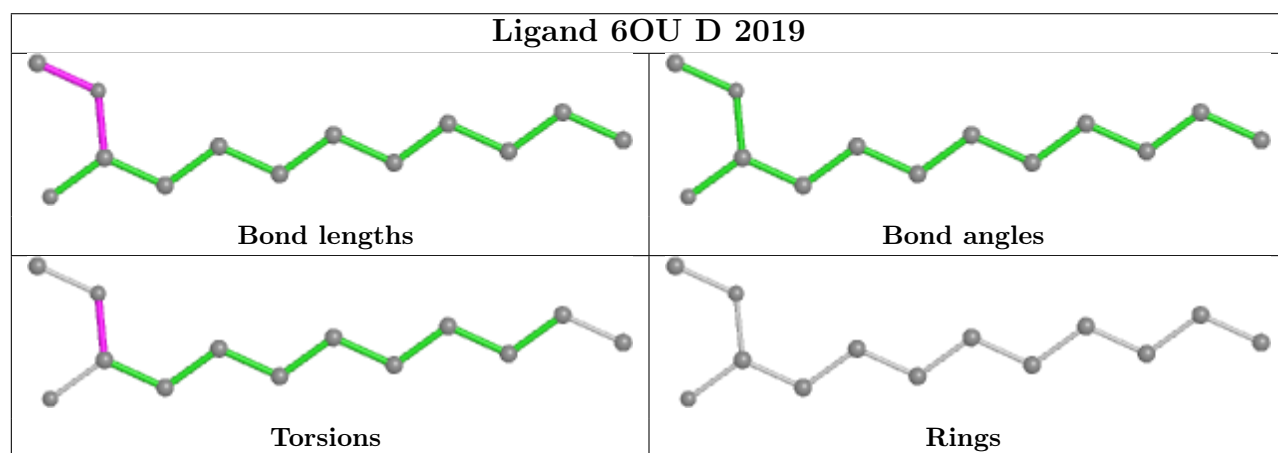
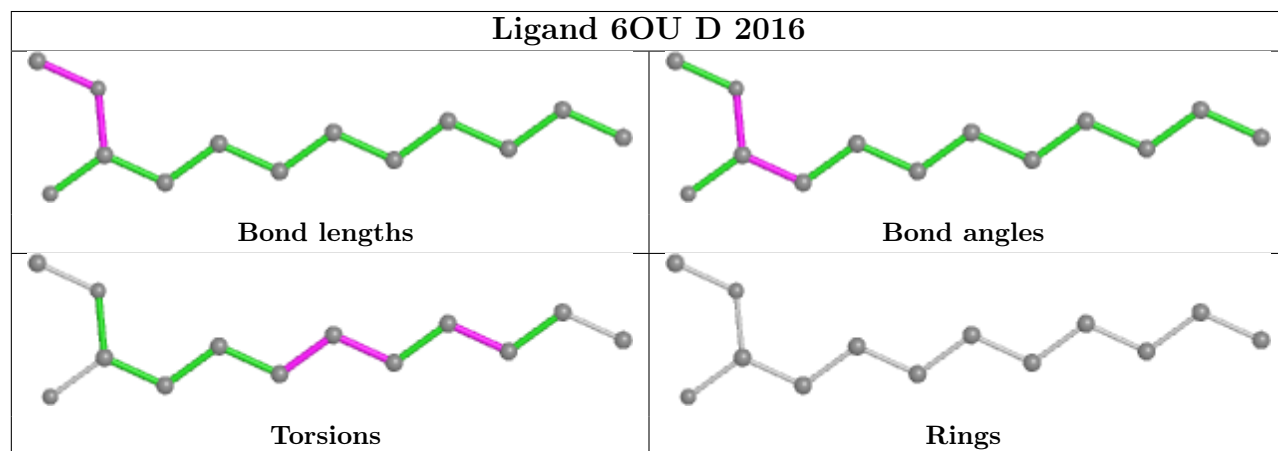
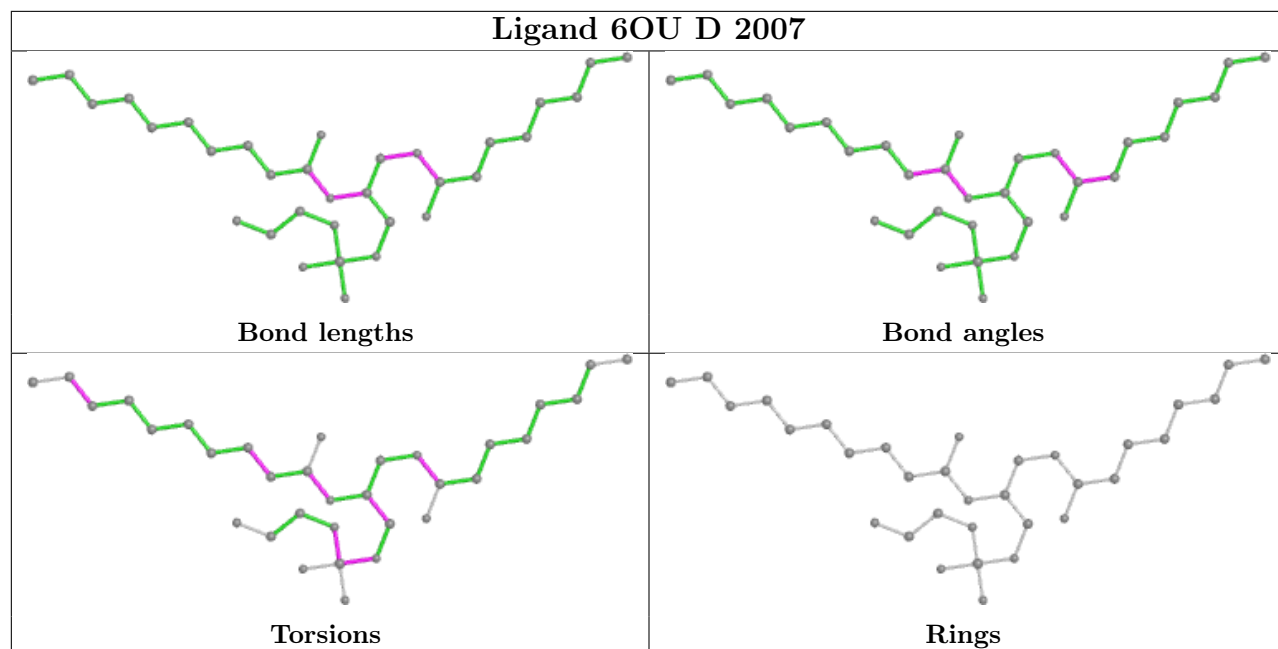
There are no ring outliers.

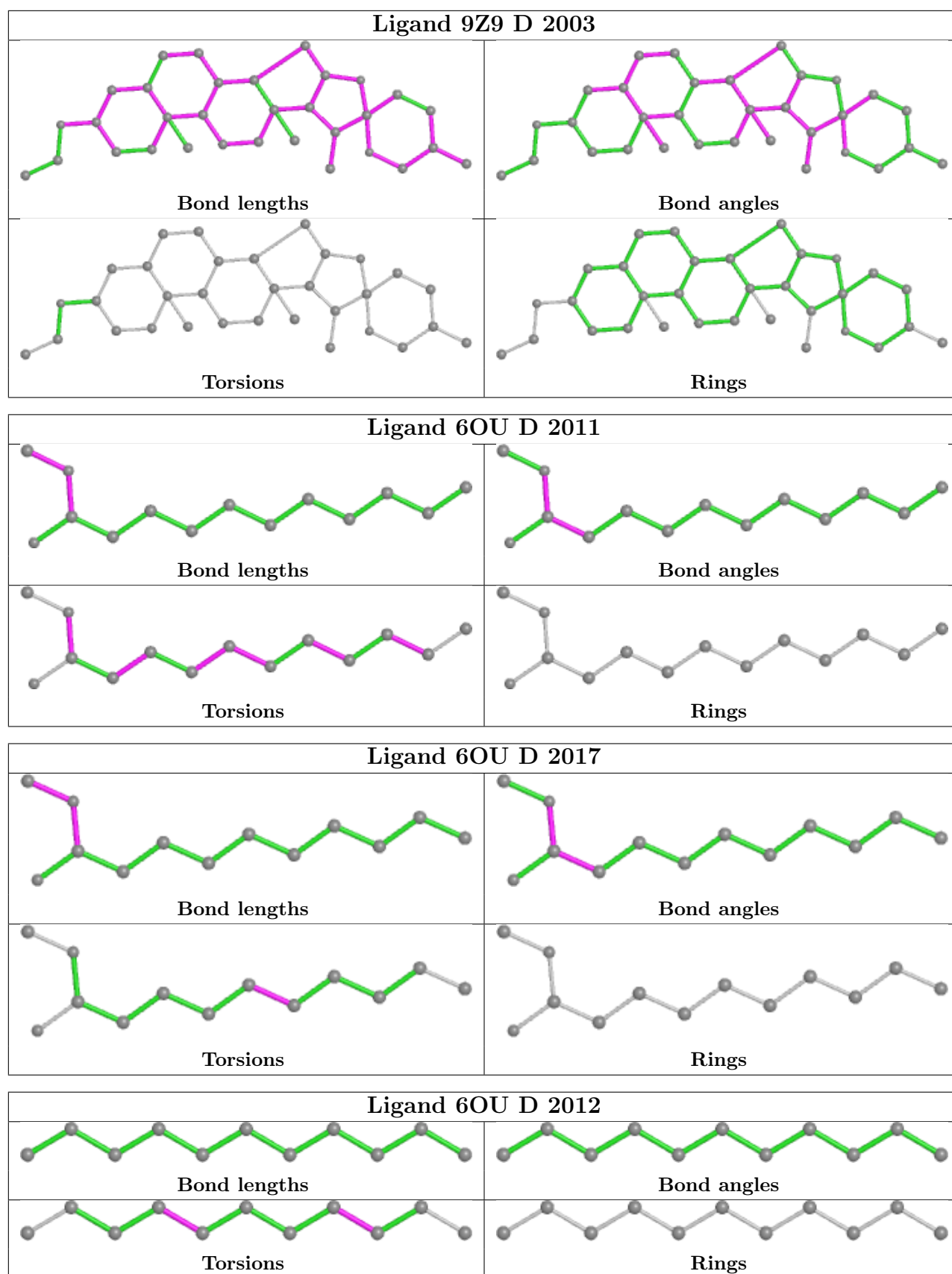
4 monomers are involved in 56 short contacts:

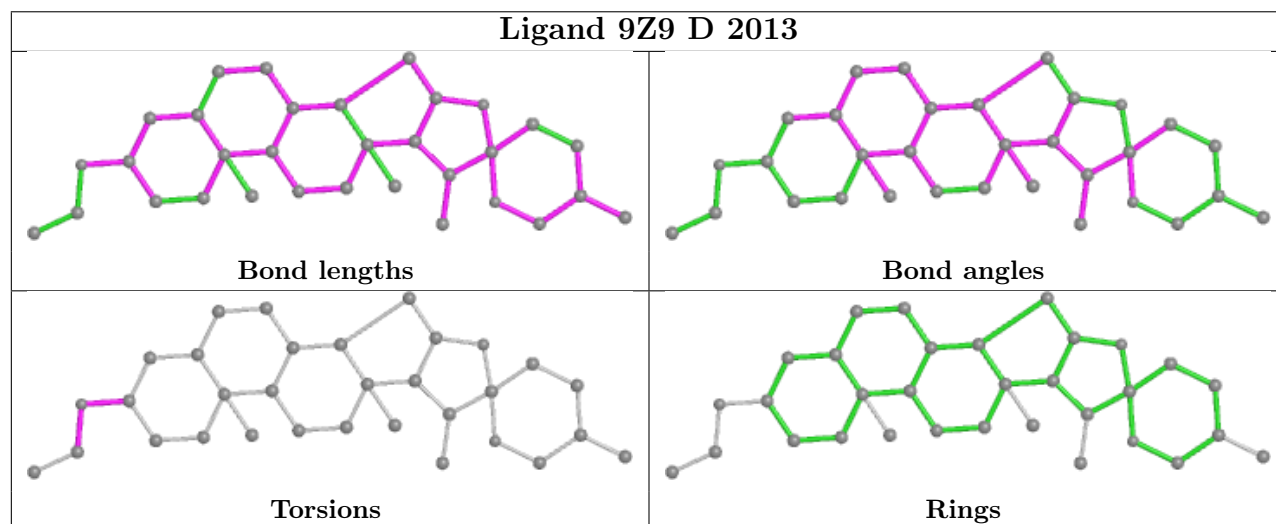
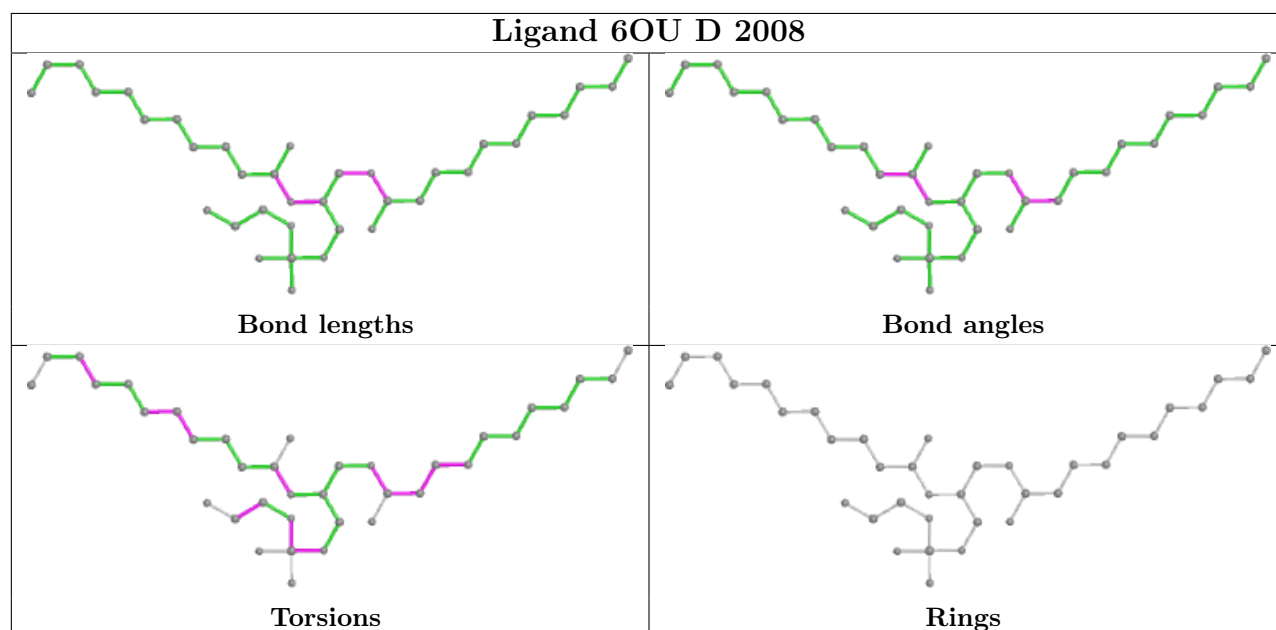
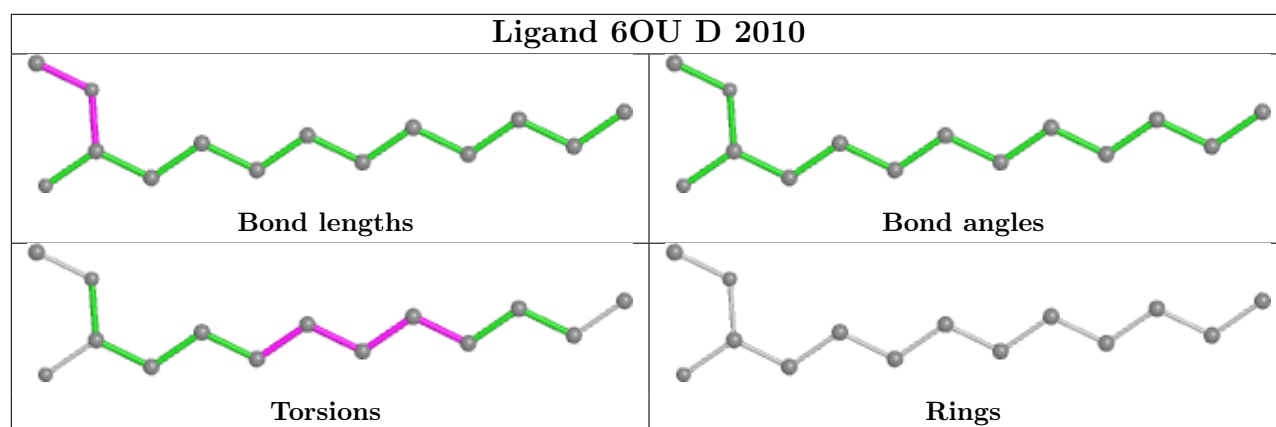
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	NAG	1	0
7	D	2003	9Z9	18	0
7	D	2013	9Z9	19	0
7	D	2002	9Z9	18	0

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.

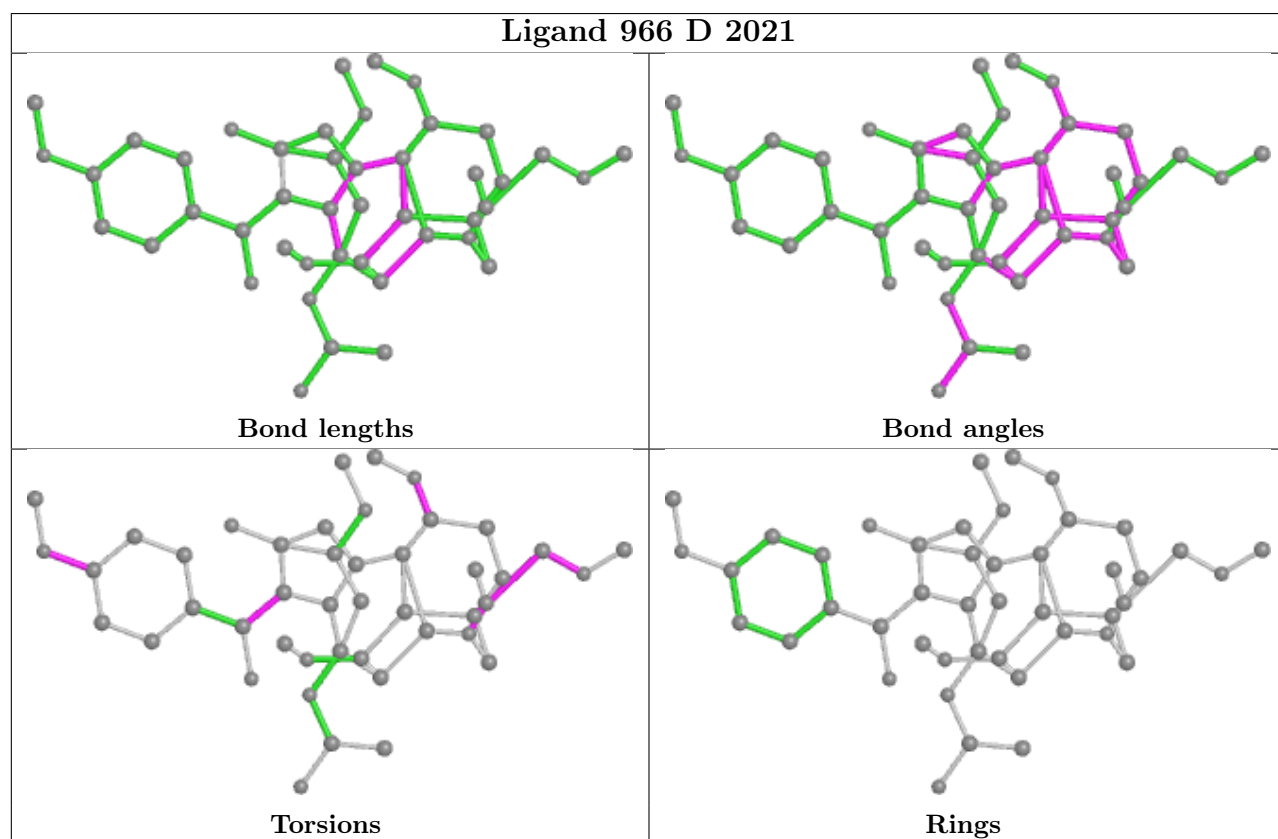
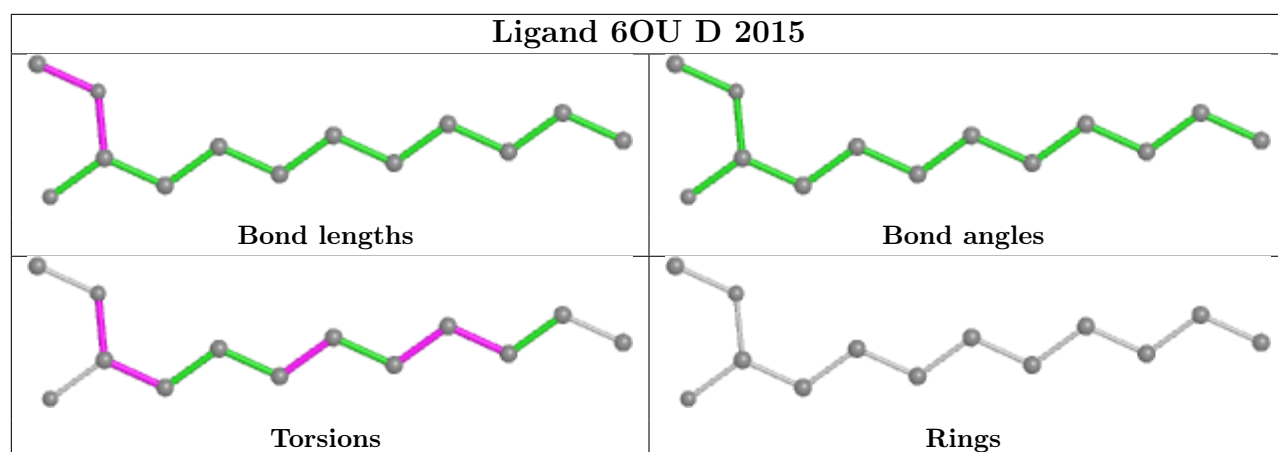


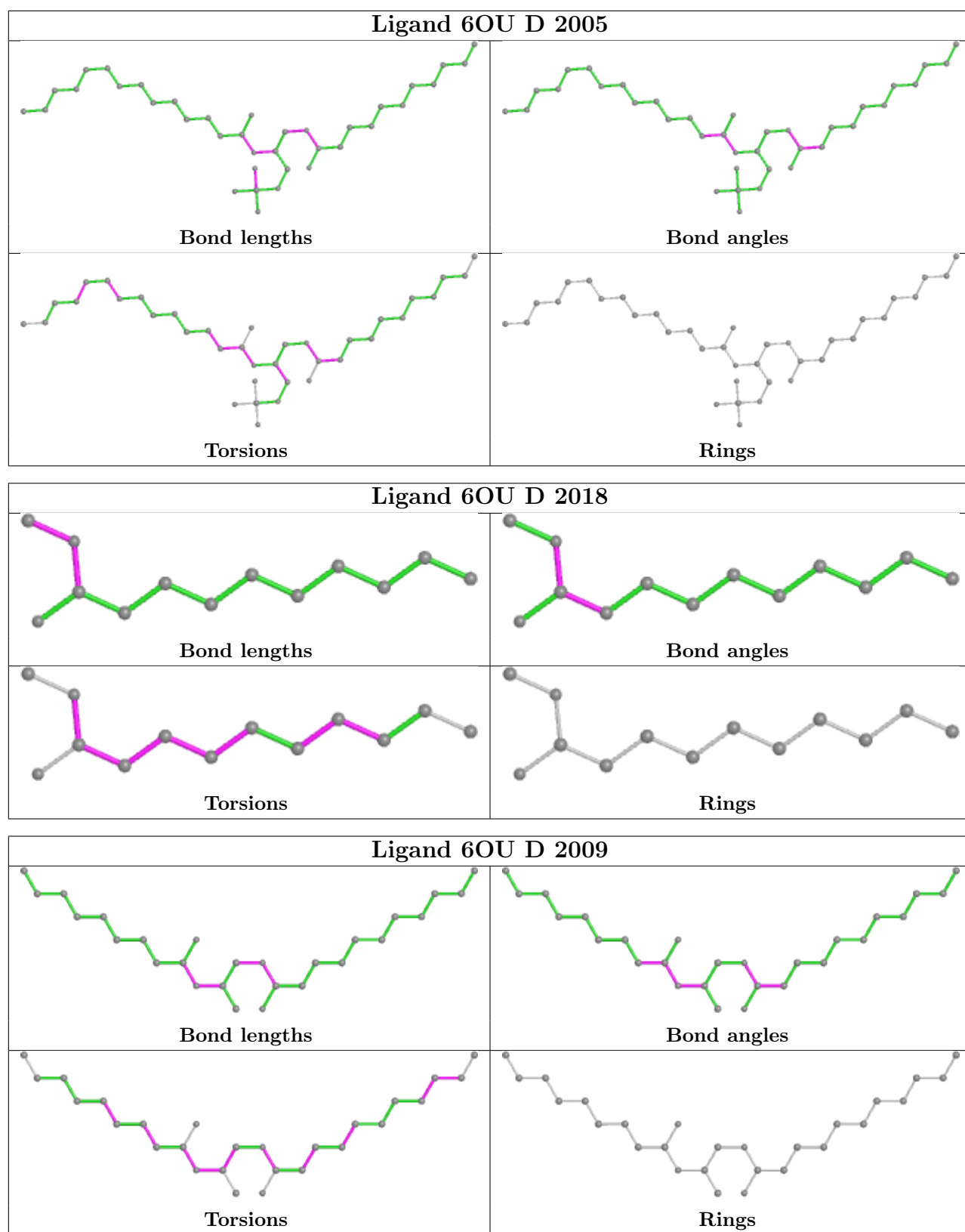


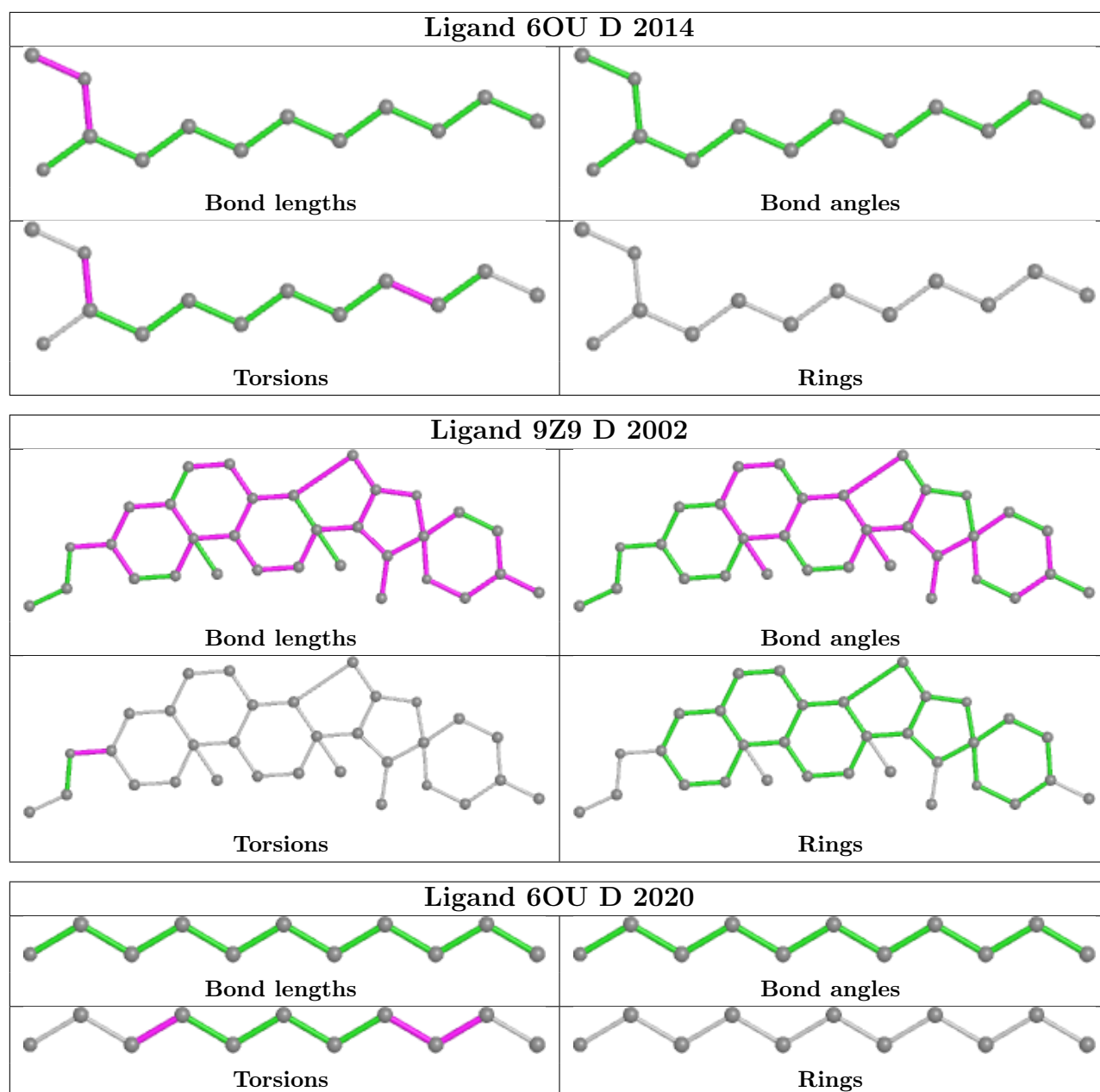












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

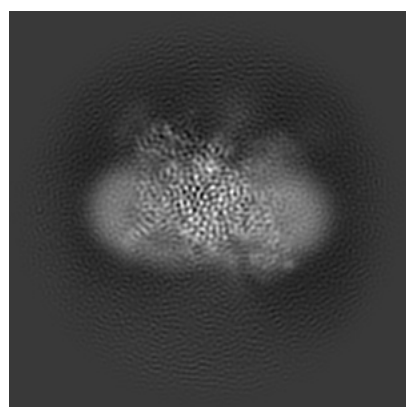
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32341. These allow visual inspection of the internal detail of the map and identification of artifacts.

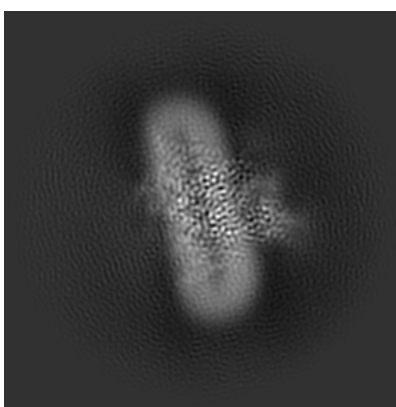
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

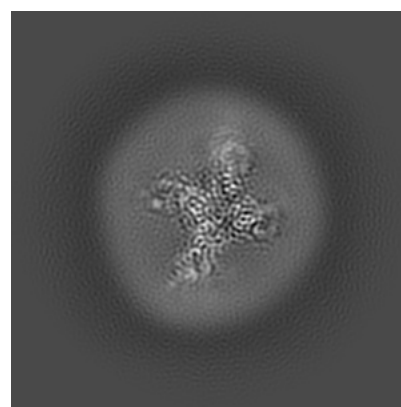
#### 6.1.1 Primary map



X



Y

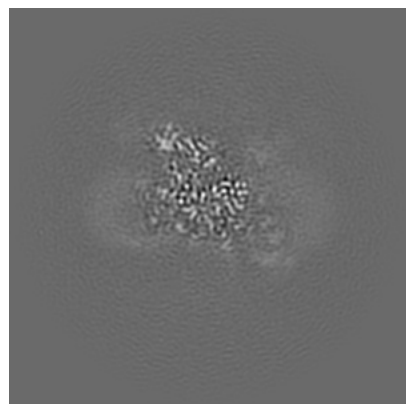


Z

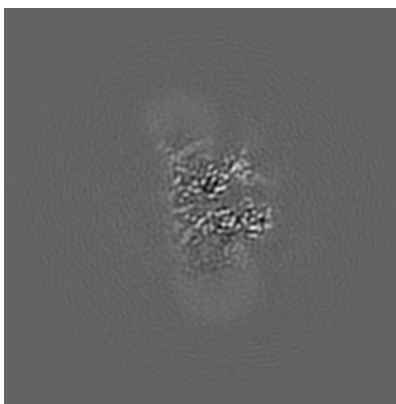
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

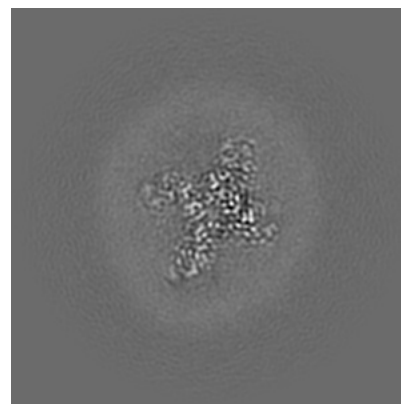
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

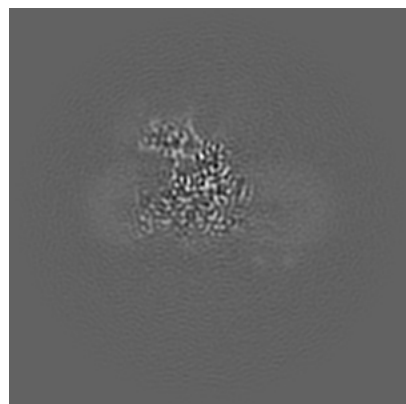


Z Index: 128

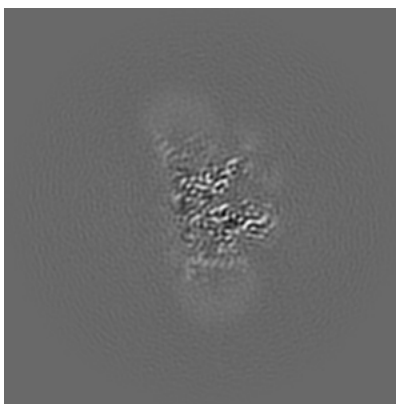
The images above show central slices of the map in three orthogonal directions.

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

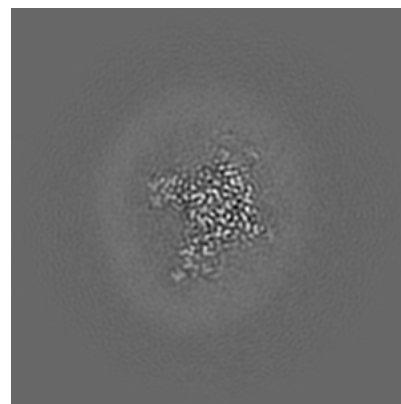
### 6.3.1 Primary map



X Index: 121



Y Index: 131

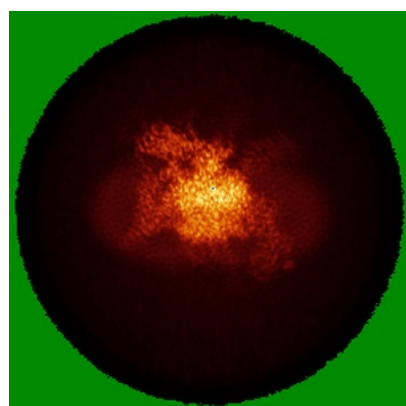


Z Index: 135

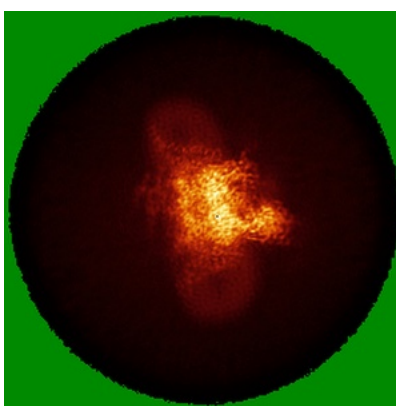
The images above show the largest variance slices of the map in three orthogonal directions.

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

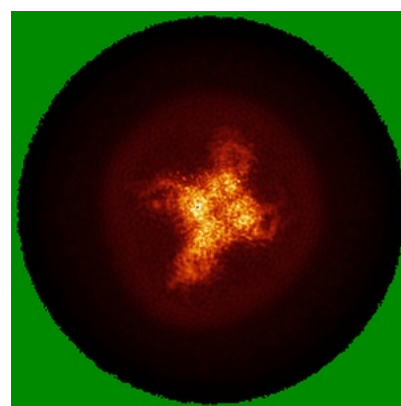
### 6.4.1 Primary map



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

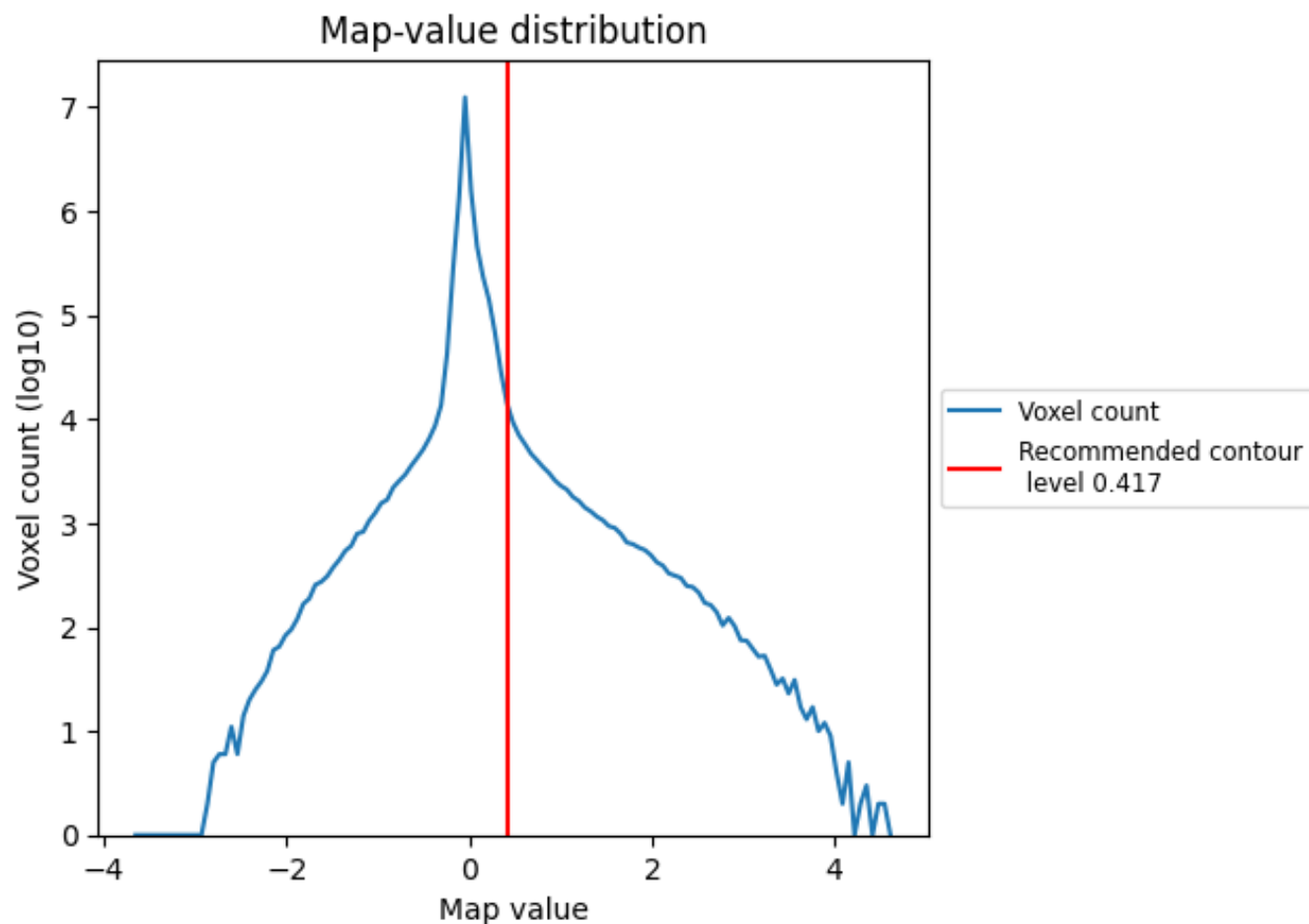
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

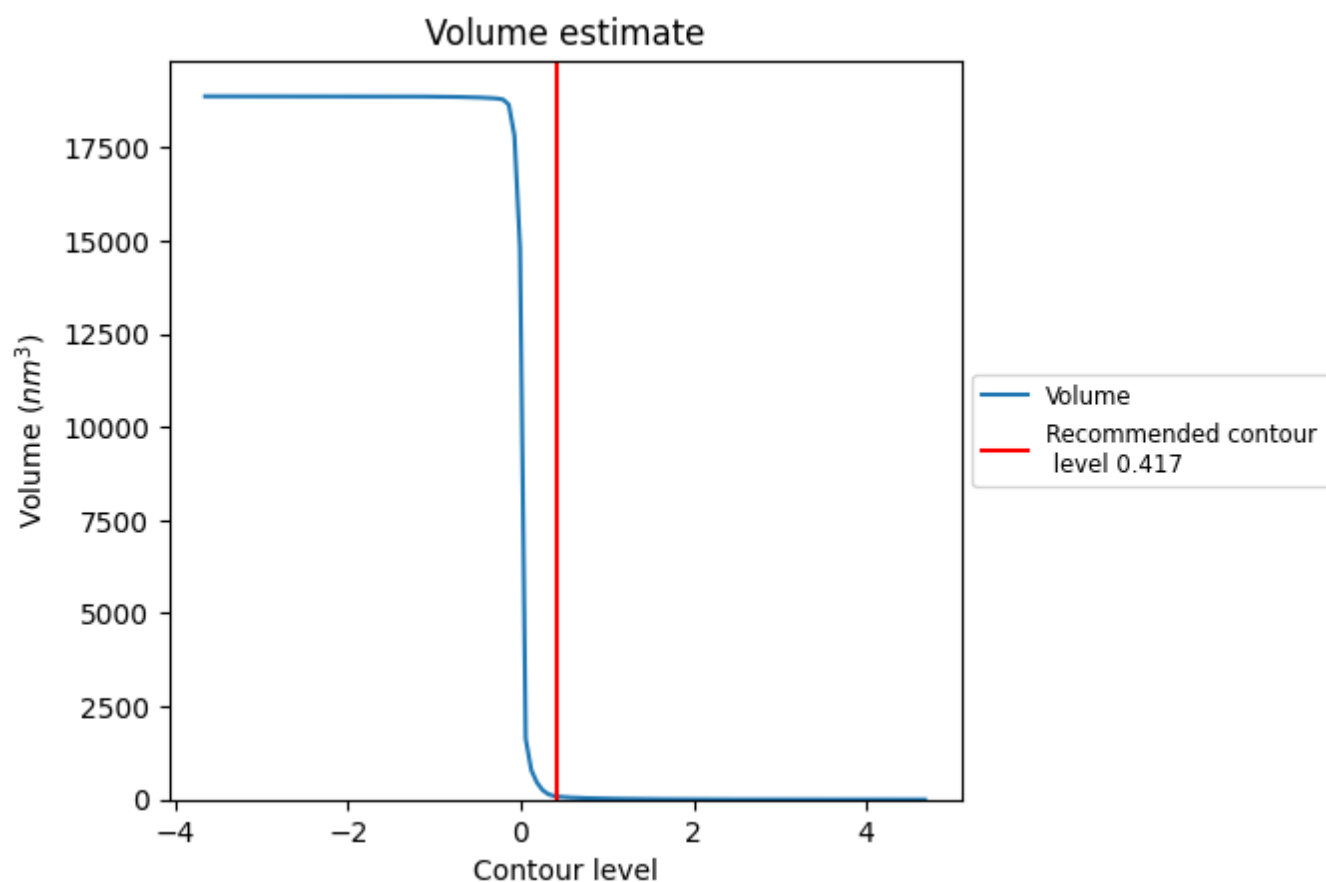
This section contains the results of statistical analysis of the map.

### 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](#)

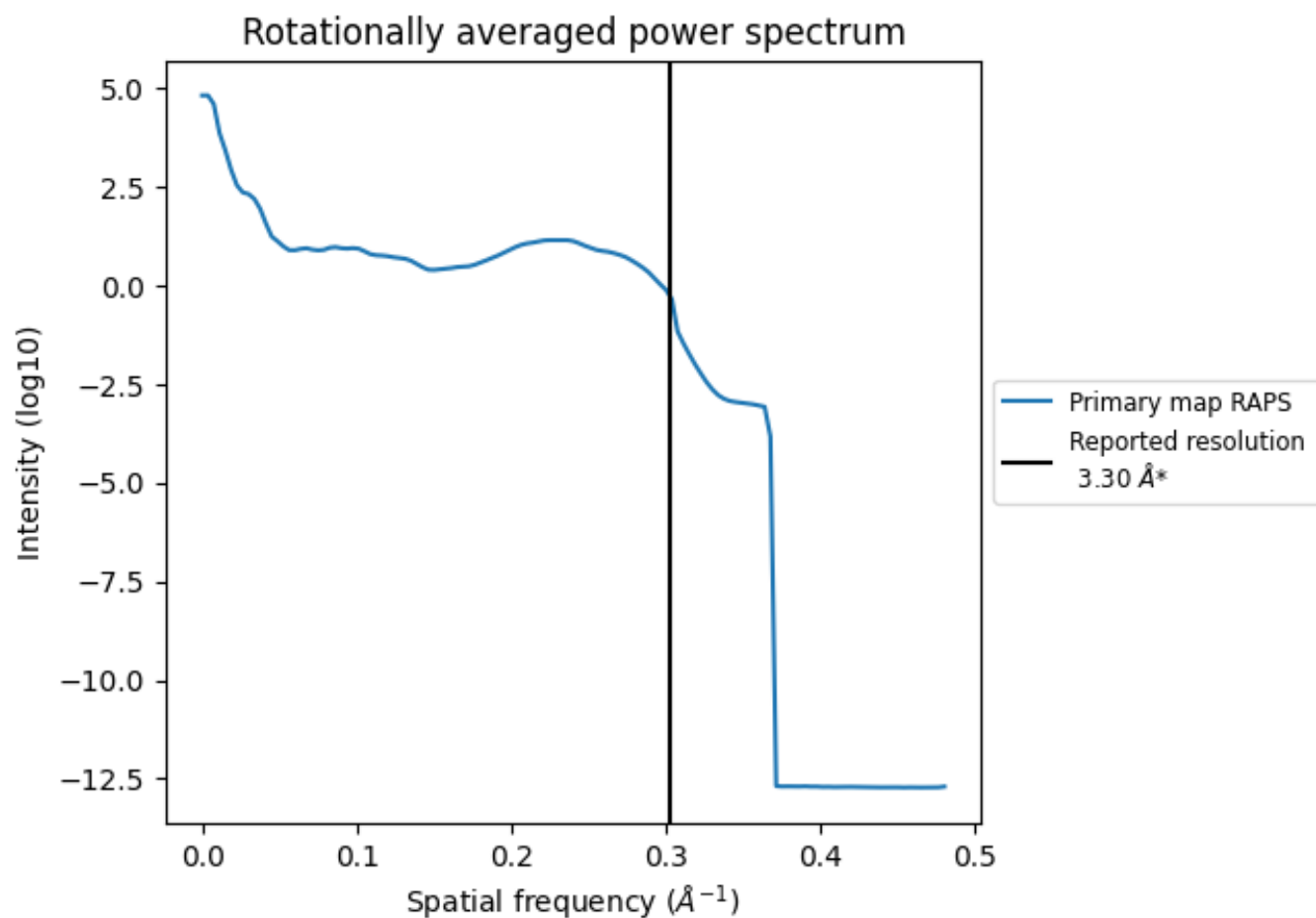


The volume at the recommended contour level is 86 nm<sup>3</sup>; this corresponds to an approximate mass of 78 kDa.

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 0.303 Å<sup>-1</sup>

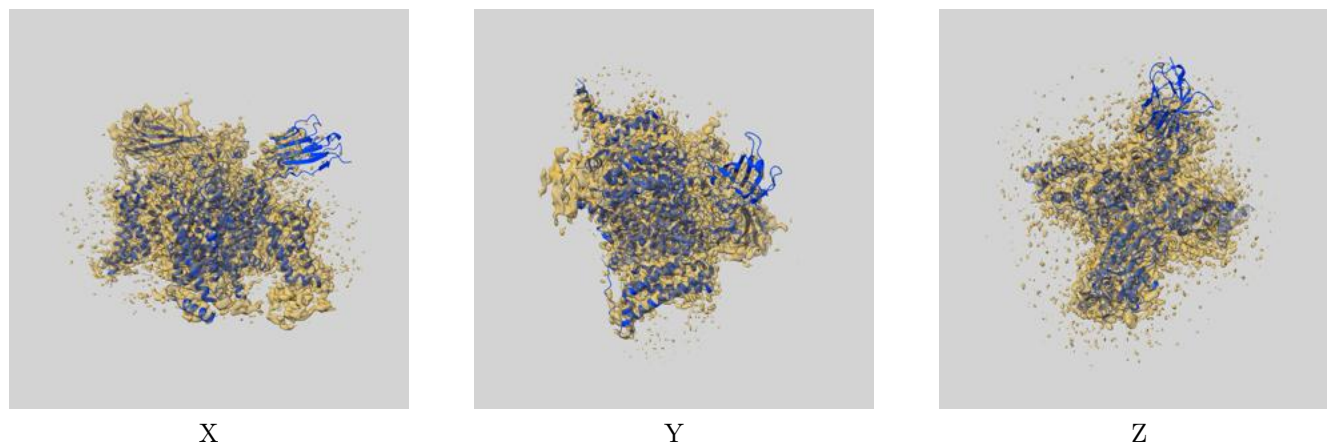
## 8 Fourier-Shell correlation

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

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

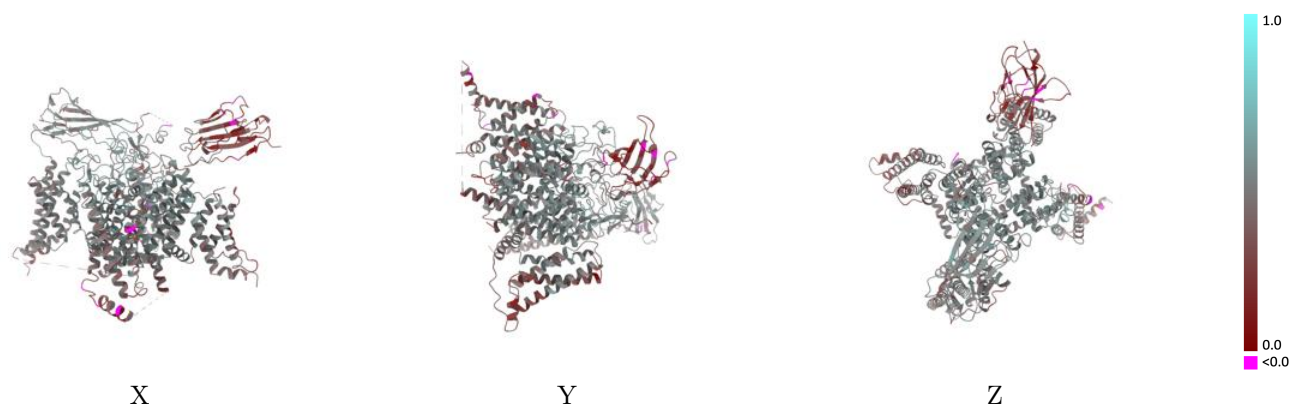
This section contains information regarding the fit between EMDB map EMD-32341 and PDB model 7W77. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.417 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



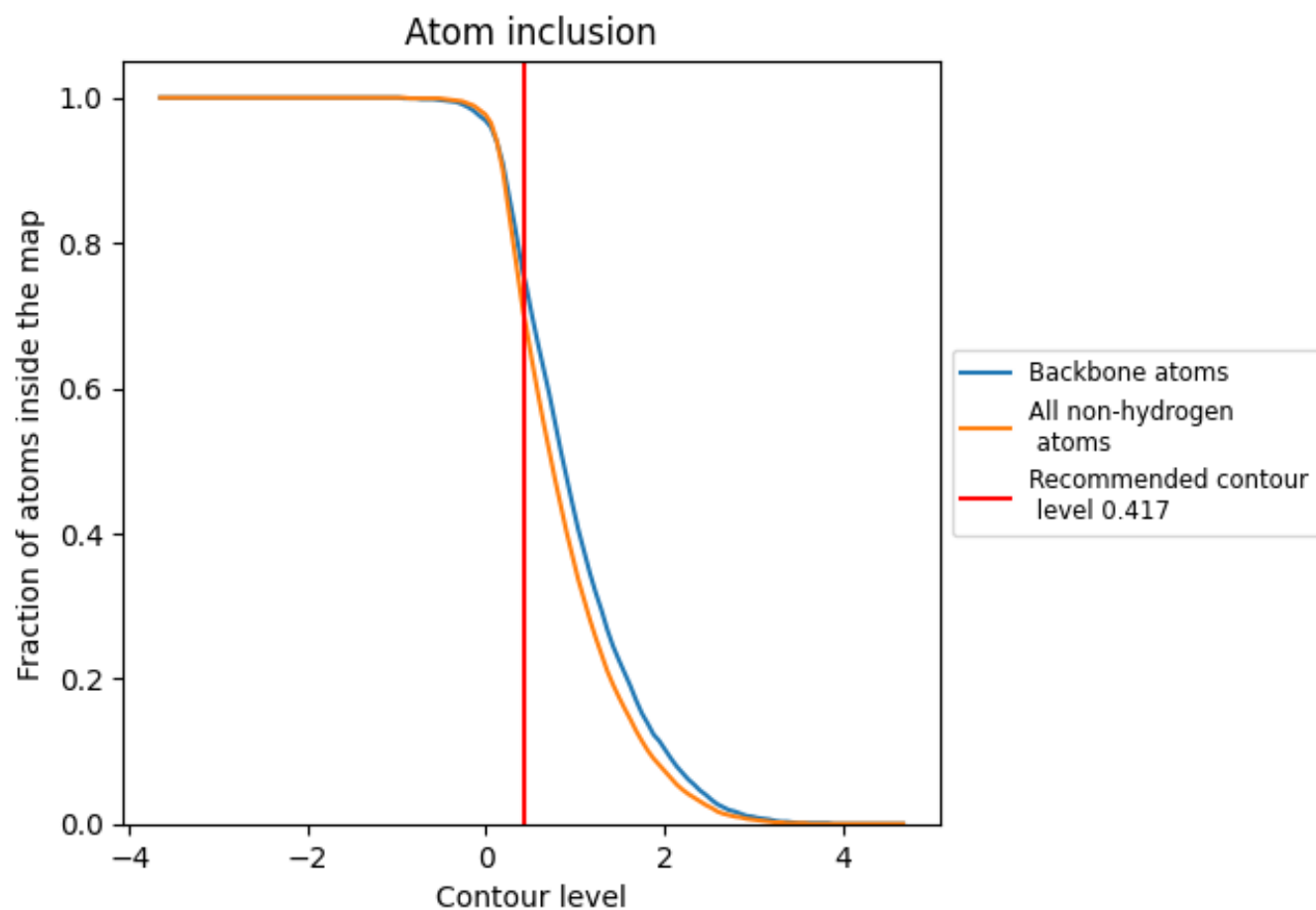
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.417).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.417) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7050	<div></div> 0.4490
B	<div></div> 0.7530	<div></div> 0.4600
C	<div></div> 0.1850	<div></div> 0.2740
D	<div></div> 0.7510	<div></div> 0.4660
E	<div></div> 0.9230	<div></div> 0.5040
F	<div></div> 0.5710	<div></div> 0.4380

