



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:54 PM BST

PDB ID : 1U19  
Title : Crystal Structure of Bovine Rhodopsin at 2.2 Angstroms Resolution  
Authors : Okada, T.; Sugihara, M.; Bondar, A.N.; Elstner, M.; Entel, P.; Buss, V.  
Deposited on : 2004-07-15  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

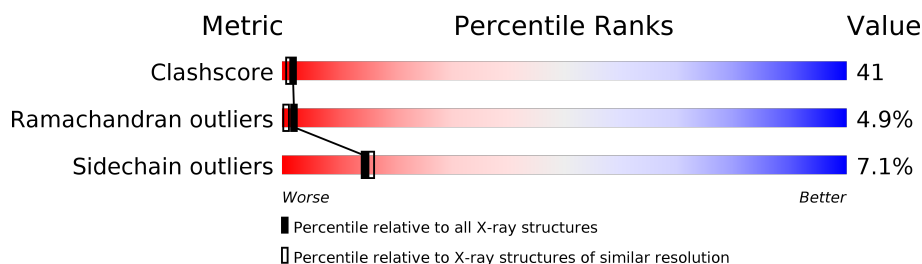
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	<div> <div>48%</div> <div>43%</div> <div>9%</div> </div>
1	B	349	<div> <div>46%</div> <div>44%</div> <div>9%</div> </div>
2	C	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div>100%</div> </div>
4	E	4	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5948 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

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



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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-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				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

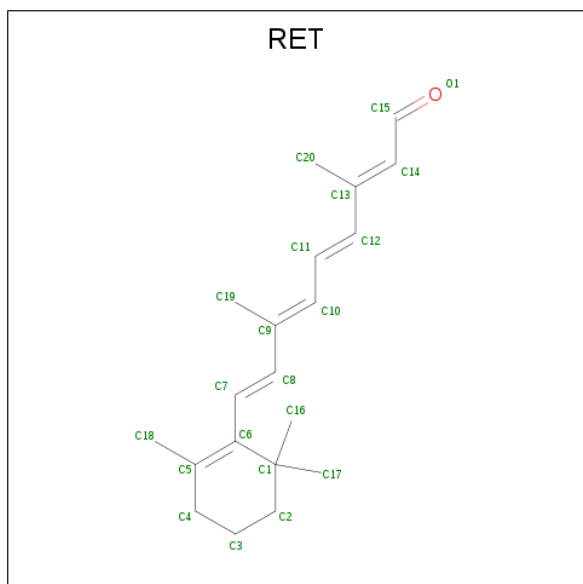
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Hg	0	0
			3	3		
5	A	3	Total	Hg	0	0
			3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

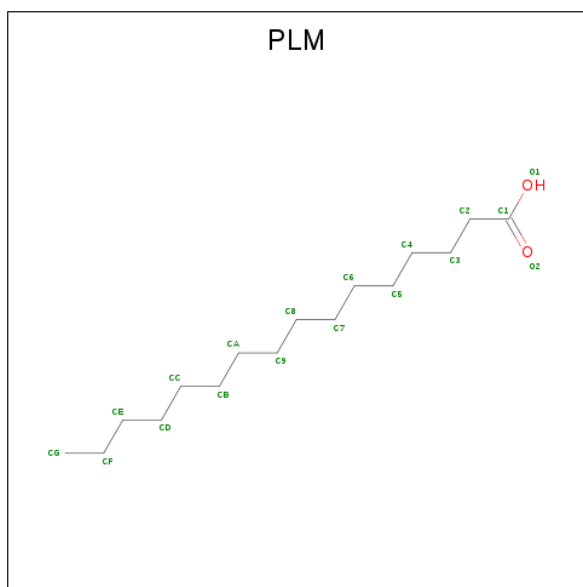
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Zn	0	0
			3	3		
6	A	4	Total	Zn	0	0
			4	4		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



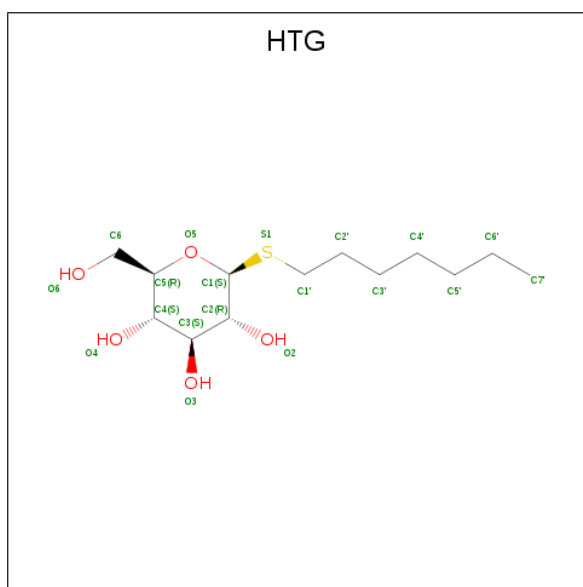
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 20 20	0	0
7	B	1	Total C 20 20	0	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



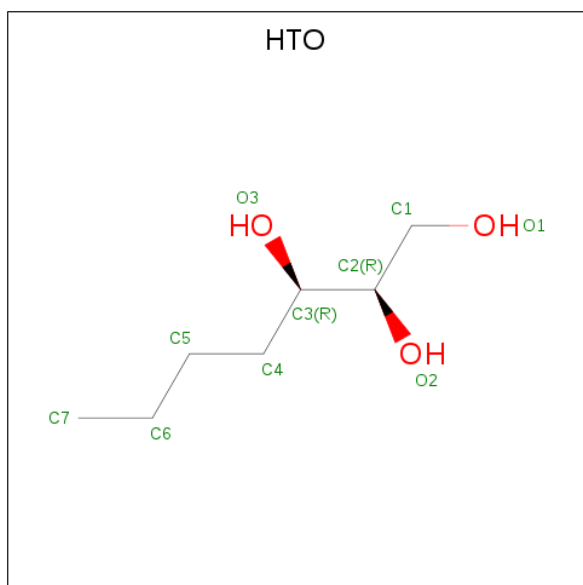
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 17 16 1	0	0
8	A	1	Total C O 17 16 1	0	0
8	A	1	Total C 16 16	0	0
8	B	1	Total C O 17 16 1	0	0
8	B	1	Total C O 17 16 1	0	0
8	B	1	Total C 16 16	0	0

- Molecule 9 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	S	0	0
			19	13	5	1		
9	B	1	Total	C	O	S	0	0
			19	13	5	1		
9	B	1	Total	C	O	S	0	0
			19	13	5	1		
9	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is water.

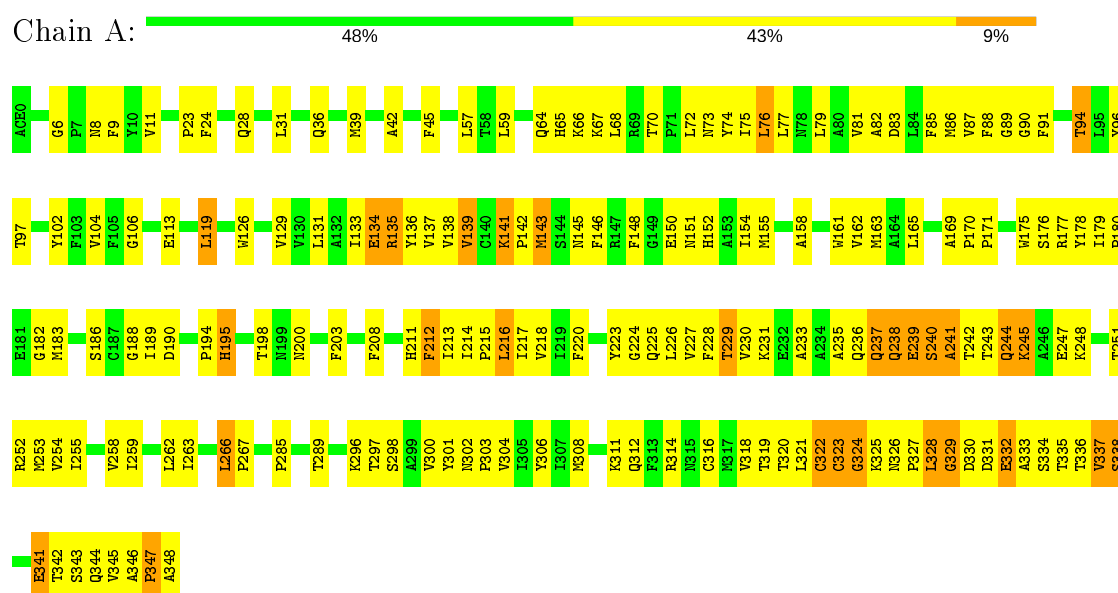
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	37	Total	O	0	0
			37	37		
11	B	29	Total	O	0	0
			29	29		

### 3 Residue-property plots

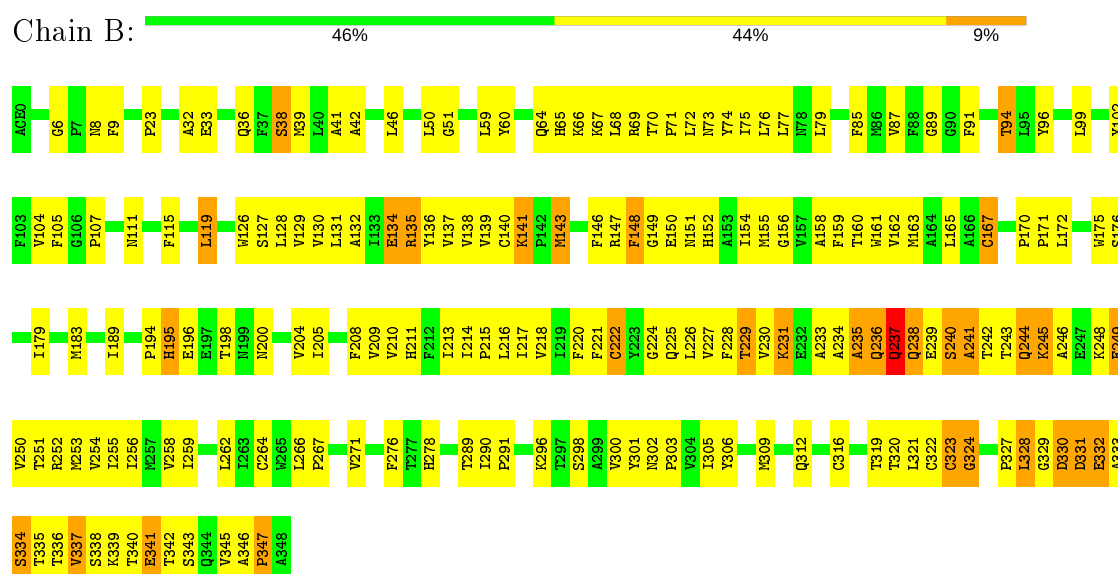
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: Rhodopsin



#### • Molecule 1: Rhodopsin





- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  33% 33% 33%

 NAG1  
NAG2  
MAN3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

 NAG1  
NAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

 NAG1  
NAG2

- Molecule 4: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

 NAG1  
NAG2  
BMA3  
BMA4

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.68 Å 96.68 Å 150.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	85.4 (50.00-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, HG, MAN

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	0.60	0/2831	0.68	1/3859 (0.0%)
1	B	0.59	0/2831	0.68	1/3859 (0.0%)
All	All	0.60	0/5662	0.68	2/7718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CD-CE-NZ	5.94	125.36	111.70
1	B	296	LYS	CD-CE-NZ	5.66	124.72	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2749	0	2706	222	1
1	B	2749	0	2706	268	0
2	C	39	0	34	1	0
3	D	28	0	25	2	0
3	F	28	0	25	0	0
4	E	50	0	43	0	0
5	A	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	3	0	0	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	20	0	27	1	0
7	B	20	0	27	0	0
8	A	50	0	89	4	0
8	B	50	0	89	5	0
9	A	19	0	26	0	0
9	B	57	0	78	3	1
10	B	10	0	16	1	0
11	A	37	0	0	3	0
11	B	29	0	0	4	0
All	All	5948	0	5891	487	1

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 41.

All (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.26	1.15
1:B:312:GLN:HA	1:B:332:GLU:HG2	1.28	1.15
1:B:239:GLU:HB2	1:B:245:LYS:HD2	1.33	1.10
1:B:337:VAL:HB	1:B:343:SER:HA	1.35	1.08
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.33	1.05
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.41	1.03
1:A:316:CYS:SG	1:A:337:VAL:HG13	2.05	0.96
1:B:245:LYS:NZ	1:B:248:LYS:HD2	1.82	0.94
1:B:230:VAL:HG23	1:B:248:LYS:HD3	1.50	0.92
1:A:326:ASN:O	1:A:328:LEU:HD22	1.71	0.91
1:A:329:GLY:HA2	1:B:96:TYR:CE1	2.05	0.90
1:A:311:LYS:HD2	1:A:314:ARG:NH2	1.87	0.90
1:A:88:PHE:HB3	8:B:1323:PLM:HB1	1.54	0.89
1:B:245:LYS:HZ3	1:B:248:LYS:HD2	1.35	0.89
1:A:341:GLU:OE1	1:A:342:THR:HG22	1.74	0.88
1:B:238:GLN:HG3	1:B:241:ALA:H	1.37	0.87
1:B:346:ALA:N	1:B:347:PRO:HD3	1.89	0.86
1:A:329:GLY:HA2	1:B:96:TYR:HE1	1.39	0.85
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.58	0.85
1:A:91:PHE:HA	1:A:94:THR:CG2	2.06	0.85
1:B:65:HIS:HB2	1:B:68:LEU:HD12	1.60	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PHE:HA	1:B:179:ILE:HD11	1.58	0.84
1:A:96:TYR:HE2	1:A:104:VAL:HG21	1.44	0.83
1:B:312:GLN:HA	1:B:332:GLU:CG	2.08	0.83
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.61	0.82
1:A:161:TRP:O	1:A:165:LEU:HD23	1.79	0.82
1:A:245:LYS:HA	1:A:245:LYS:HZ2	1.44	0.82
1:B:239:GLU:HB3	1:B:244:GLN:HE22	1.45	0.82
1:B:67:LYS:HZ2	1:B:312:GLN:HG3	1.42	0.81
1:B:91:PHE:HA	1:B:94:THR:CG2	2.09	0.81
1:A:239:GLU:HB3	1:A:244:GLN:CD	2.01	0.81
1:B:161:TRP:O	1:B:165:LEU:HD23	1.79	0.81
1:B:67:LYS:NZ	1:B:312:GLN:HG3	1.96	0.81
1:A:65:HIS:ND1	1:A:338:SER:HA	1.96	0.80
1:B:67:LYS:HD3	1:B:337:VAL:HG13	1.64	0.80
1:B:337:VAL:HG23	1:B:338:SER:N	1.94	0.80
1:A:341:GLU:HG3	1:A:342:THR:N	1.97	0.80
1:B:75:ILE:HG13	1:B:131:LEU:CD1	2.11	0.80
1:A:65:HIS:HB3	1:A:337:VAL:CG2	2.11	0.80
1:B:38:SER:HB3	9:B:1508:HTG:H4'1	1.62	0.79
1:A:341:GLU:CG	1:A:342:THR:H	1.94	0.79
1:B:136:TYR:HA	1:B:226:LEU:HD11	1.64	0.78
1:A:70:THR:H	1:A:73:ASN:HD22	1.32	0.78
1:B:139:VAL:HG11	1:B:230:VAL:HG12	1.66	0.77
1:B:322:CYS:HA	8:B:1322:PLM:O2	1.85	0.77
1:A:325:LYS:HE3	1:A:341:GLU:OE1	1.85	0.77
1:B:234:ALA:HB1	1:B:245:LYS:HE2	1.67	0.77
1:A:341:GLU:HG3	1:A:342:THR:H	1.50	0.77
1:A:245:LYS:HA	1:A:245:LYS:NZ	2.01	0.76
1:A:326:ASN:HD21	1:A:328:LEU:HD11	1.49	0.76
1:B:271:VAL:HG21	1:B:291:PRO:HG3	1.68	0.75
1:B:332:GLU:HB3	1:B:335:THR:O	1.86	0.75
1:A:239:GLU:HB3	1:A:244:GLN:OE1	1.87	0.74
1:B:69:ARG:N	1:B:73:ASN:HD22	1.86	0.74
1:A:308:MET:HE3	1:B:99:LEU:HD21	1.68	0.74
1:A:332:GLU:C	1:A:334:SER:H	1.89	0.74
1:B:70:THR:H	1:B:73:ASN:ND2	1.86	0.74
1:A:150:GLU:O	1:A:154:ILE:HG13	1.86	0.74
1:B:337:VAL:HA	1:B:342:THR:O	1.87	0.74
1:B:139:VAL:CG1	1:B:230:VAL:HG12	2.17	0.74
1:A:239:GLU:HG2	1:A:248:LYS:NZ	2.02	0.74
1:B:183:MET:HE3	1:B:289:THR:HG21	1.70	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:H	1:B:73:ASN:HD22	1.37	0.73
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.69	0.73
1:A:65:HIS:CG	1:A:338:SER:HA	2.23	0.73
1:B:239:GLU:HB2	1:B:245:LYS:CD	2.17	0.72
1:B:337:VAL:HA	1:B:342:THR:C	2.10	0.72
1:A:137:VAL:O	1:A:141:LYS:HA	1.87	0.72
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.70	0.72
1:B:75:ILE:HG13	1:B:131:LEU:HD11	1.70	0.72
1:A:65:HIS:ND1	1:A:337:VAL:O	2.18	0.72
1:B:234:ALA:HA	1:B:245:LYS:NZ	2.05	0.72
1:B:267:PRO:HG2	11:B:2019:HOH:O	1.89	0.72
1:A:59:LEU:HD12	1:A:77:LEU:HD11	1.72	0.71
1:B:237:GLN:O	1:B:238:GLN:HB3	1.90	0.71
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.72	0.71
1:A:308:MET:CE	1:B:99:LEU:HD21	2.20	0.71
1:B:245:LYS:HE3	1:B:245:LYS:CA	2.15	0.70
1:B:65:HIS:CG	1:B:338:SER:HA	2.27	0.70
1:B:208:PHE:O	1:B:213:ILE:HG13	1.91	0.70
1:B:238:GLN:HA	1:B:242:THR:HA	1.73	0.70
1:A:212:PHE:O	1:A:216:LEU:HD23	1.92	0.70
1:B:132:ALA:O	1:B:222:CYS:SG	2.50	0.69
1:B:59:LEU:HD13	1:B:77:LEU:HD11	1.74	0.69
1:B:278:HIS:NE2	11:B:2038:HOH:O	2.23	0.69
1:A:59:LEU:CD1	1:A:77:LEU:HD11	2.22	0.69
1:B:230:VAL:HG23	1:B:248:LYS:CD	2.22	0.69
1:A:96:TYR:HE2	1:A:104:VAL:CG2	2.06	0.69
1:A:148:PHE:HA	1:A:152:HIS:ND1	2.08	0.69
1:B:238:GLN:HG3	1:B:241:ALA:N	2.07	0.69
1:A:135:ARG:NE	1:A:135:ARG:HA	2.08	0.68
1:A:337:VAL:O	1:A:338:SER:OG	2.11	0.68
1:A:304:VAL:O	1:A:308:MET:HG2	1.94	0.68
1:B:67:LYS:HB3	1:B:337:VAL:CG1	2.24	0.67
1:A:183:MET:HE3	1:A:289:THR:HG21	1.77	0.67
1:A:325:LYS:HE2	1:A:327:PRO:HD3	1.76	0.67
1:A:239:GLU:HB3	1:A:244:GLN:NE2	2.10	0.67
1:B:46:LEU:HD12	8:B:1407:PLM:HD2	1.77	0.67
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.76	0.67
1:B:9:PHE:CA	1:B:179:ILE:HD11	2.23	0.67
1:B:67:LYS:N	1:B:337:VAL:HG21	2.10	0.67
1:B:338:SER:HB2	1:B:341:GLU:HG3	1.75	0.66
1:A:341:GLU:CG	1:A:342:THR:N	2.58	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:NZ	1:B:233:ALA:HB3	2.10	0.66
1:B:59:LEU:HA	1:B:77:LEU:CD1	2.26	0.66
1:A:76:LEU:HD22	1:A:306:TYR:CG	2.30	0.66
1:B:167:CYS:O	1:B:170:PRO:HD2	1.95	0.66
1:A:322:CYS:O	1:A:324:GLY:N	2.28	0.65
1:B:239:GLU:HB3	1:B:244:GLN:NE2	2.10	0.65
1:B:338:SER:HB2	1:B:341:GLU:CG	2.26	0.65
1:A:312:GLN:HB2	1:A:332:GLU:HG3	1.79	0.65
1:B:143:MET:HA	1:B:143:MET:CE	2.27	0.65
1:B:67:LYS:HZ3	1:B:335:THR:C	2.00	0.65
1:A:311:LYS:NZ	1:A:330:ASP:HB2	2.12	0.65
1:A:230:VAL:HG23	1:A:248:LYS:HE2	1.78	0.65
1:B:67:LYS:HB3	1:B:337:VAL:HG11	1.79	0.64
1:B:255:ILE:O	1:B:259:ILE:HG12	1.97	0.64
1:B:64:GLN:HG2	1:B:65:HIS:CD2	2.32	0.64
1:A:338:SER:HB2	1:A:341:GLU:HG2	1.78	0.64
1:A:198:THR:HG23	1:A:200:ASN:OD1	1.98	0.64
1:B:59:LEU:CD1	1:B:77:LEU:HD11	2.28	0.64
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.33	0.64
1:B:67:LYS:HB3	1:B:337:VAL:CG2	2.28	0.63
1:B:129:VAL:HG13	1:B:218:VAL:HG11	1.80	0.63
1:A:321:LEU:HD13	8:A:1322:PLM:H72	1.81	0.63
1:B:209:VAL:O	1:B:214:ILE:HG13	1.99	0.63
1:B:235:ALA:HB3	1:B:239:GLU:OE1	1.98	0.63
1:A:239:GLU:HG2	1:A:248:LYS:HZ2	1.61	0.62
1:B:337:VAL:HA	1:B:342:THR:HG23	1.82	0.62
1:B:337:VAL:CA	1:B:342:THR:HG23	2.29	0.62
1:A:129:VAL:HG13	1:A:218:VAL:HG11	1.81	0.62
2:C:1:NAG:H61	2:C:2:NAG:C7	2.29	0.62
1:A:345:VAL:HG12	1:A:347:PRO:CD	2.25	0.61
1:B:127:SER:O	1:B:131:LEU:HD13	2.00	0.61
1:A:325:LYS:HG2	1:A:327:PRO:HD3	1.83	0.61
1:B:67:LYS:H	1:B:337:VAL:HG21	1.66	0.61
1:B:91:PHE:HA	1:B:94:THR:HG22	1.82	0.61
1:A:75:ILE:HG21	1:A:131:LEU:HD11	1.81	0.60
1:B:9:PHE:HA	1:B:179:ILE:CD1	2.29	0.60
1:A:321:LEU:HD13	8:A:1322:PLM:H51	1.83	0.60
1:B:298:SER:HA	1:B:301:TYR:CE2	2.36	0.60
1:A:198:THR:CG2	1:A:200:ASN:OD1	2.49	0.60
1:B:135:ARG:HD3	1:B:251:THR:HA	1.83	0.60
1:B:194:PRO:O	1:B:195:HIS:C	2.40	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG13	1:A:228:PHE:N	2.15	0.60
1:A:342:THR:O	1:A:342:THR:HG23	2.01	0.60
1:A:65:HIS:HB2	1:A:68:LEU:HD12	1.84	0.60
1:A:75:ILE:HG13	1:A:131:LEU:CD1	2.32	0.60
1:B:67:LYS:HB3	1:B:337:VAL:HG21	1.84	0.60
1:A:235:ALA:HB3	1:A:239:GLU:OE1	2.01	0.59
1:A:139:VAL:HG11	1:A:226:LEU:HG	1.83	0.59
1:B:64:GLN:HG2	1:B:65:HIS:HD2	1.66	0.59
1:B:67:LYS:NZ	1:B:332:GLU:HG3	2.17	0.59
1:A:254:VAL:O	1:A:258:VAL:HG23	2.01	0.59
1:B:67:LYS:H	1:B:337:VAL:CG2	2.15	0.59
1:B:51:GLY:HA2	1:B:300:VAL:HG12	1.84	0.59
1:A:300:VAL:O	1:A:303:PRO:HD2	2.02	0.59
1:B:226:LEU:HD12	1:B:226:LEU:N	2.18	0.59
1:A:67:LYS:HB2	1:A:337:VAL:CB	2.31	0.59
1:B:345:VAL:C	1:B:347:PRO:HD3	2.23	0.59
1:B:159:PHE:O	1:B:163:MET:HG2	2.03	0.59
1:A:321:LEU:C	1:A:323:CYS:H	2.04	0.58
1:A:67:LYS:H	1:A:337:VAL:CG2	2.16	0.58
1:B:221:PHE:O	1:B:224:GLY:N	2.32	0.58
1:A:239:GLU:OE2	1:A:248:LYS:HD2	2.04	0.58
1:B:183:MET:CE	1:B:289:THR:HG21	2.33	0.58
8:B:1322:PLM:H52	8:B:1323:PLM:H61	1.86	0.58
1:B:239:GLU:CB	1:B:244:GLN:HE22	2.14	0.58
1:B:158:ALA:O	1:B:162:VAL:HG23	2.03	0.58
1:A:267:PRO:HG2	11:A:964:HOH:O	2.03	0.58
1:B:337:VAL:CB	1:B:343:SER:HA	2.22	0.58
1:B:337:VAL:CG2	1:B:338:SER:N	2.64	0.58
1:A:302:ASN:HB2	1:A:303:PRO:HD3	1.86	0.58
1:A:244:GLN:OE1	1:A:244:GLN:C	2.43	0.57
1:A:239:GLU:CG	1:A:244:GLN:HE22	2.16	0.57
1:A:90:GLY:O	1:A:94:THR:HG22	2.03	0.57
1:B:75:ILE:O	1:B:79:LEU:HD13	2.04	0.57
1:A:176:SER:HA	1:A:200:ASN:OD1	2.05	0.57
1:A:65:HIS:HD1	1:A:337:VAL:C	2.08	0.57
1:A:311:LYS:HD2	1:A:314:ARG:HH21	1.68	0.57
1:B:341:GLU:HG3	1:B:342:THR:H	1.70	0.57
1:A:302:ASN:HB2	11:A:2017:HOH:O	2.04	0.56
1:B:143:MET:HA	1:B:143:MET:HE2	1.86	0.56
8:A:1410:PLM:H81	1:B:46:LEU:HD11	1.86	0.56
1:B:67:LYS:HG2	1:B:337:VAL:HG22	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:HA	1:B:245:LYS:HZ2	1.71	0.56
1:B:216:LEU:HD11	1:B:262:LEU:HD21	1.87	0.56
1:B:300:VAL:O	1:B:303:PRO:HD2	2.06	0.56
1:A:251:THR:O	1:A:255:ILE:HG13	2.06	0.56
1:B:195:HIS:HD1	1:B:198:THR:CG2	2.19	0.56
1:A:91:PHE:HA	1:A:94:THR:HG22	1.88	0.55
1:B:332:GLU:CB	1:B:335:THR:O	2.55	0.55
1:A:152:HIS:O	1:A:155:MET:HB2	2.06	0.55
1:A:245:LYS:CA	1:A:245:LYS:NZ	2.70	0.55
1:A:338:SER:CB	1:A:341:GLU:HG2	2.37	0.55
1:B:332:GLU:H	1:B:336:THR:HG22	1.71	0.55
1:B:337:VAL:HB	1:B:343:SER:CA	2.24	0.55
1:B:64:GLN:HG3	1:B:339:LYS:HB2	1.88	0.55
1:B:96:TYR:HE2	1:B:104:VAL:CG2	2.20	0.55
1:A:74:TYR:CE2	1:A:150:GLU:HG2	2.42	0.54
1:B:319:THR:HG21	1:B:341:GLU:OE1	2.07	0.54
1:B:64:GLN:HA	1:B:339:LYS:HD3	1.89	0.54
1:A:91:PHE:HA	1:A:94:THR:HG23	1.87	0.54
1:B:23:PRO:O	1:B:102:TYR:HB2	2.08	0.54
1:A:237:GLN:CD	1:A:237:GLN:H	2.11	0.54
1:B:156:GLY:O	1:B:160:THR:HG23	2.08	0.54
1:B:327:PRO:HB2	1:B:331:ASP:OD2	2.07	0.54
1:B:322:CYS:O	1:B:324:GLY:N	2.41	0.54
1:B:346:ALA:N	1:B:347:PRO:CD	2.67	0.54
3:D:1:NAG:H61	3:D:2:NAG:H82	1.90	0.53
1:B:216:LEU:HD12	1:B:220:PHE:HE2	1.73	0.53
1:B:51:GLY:CA	1:B:300:VAL:HG12	2.39	0.53
1:A:311:LYS:HD2	1:A:314:ARG:HH22	1.71	0.53
1:B:143:MET:HG2	1:B:146:PHE:CB	2.38	0.53
1:B:332:GLU:O	1:B:333:ALA:HB3	2.07	0.53
1:B:216:LEU:HD12	1:B:220:PHE:CE2	2.43	0.53
1:B:237:GLN:O	1:B:238:GLN:CB	2.56	0.53
1:B:246:ALA:O	1:B:249:GLU:HG2	2.08	0.53
1:B:147:ARG:HH21	1:B:149:GLY:HA2	1.73	0.53
1:B:126:TRP:CE2	1:B:163:MET:HB3	2.43	0.53
1:B:332:GLU:HB2	1:B:336:THR:HG22	1.91	0.53
1:A:189:ILE:HG22	1:A:190:ASP:N	2.24	0.53
1:A:262:LEU:HB3	1:A:266:LEU:CD2	2.39	0.53
1:A:183:MET:CE	1:A:289:THR:HG21	2.38	0.53
1:A:88:PHE:HB2	8:B:1323:PLM:HF2	1.90	0.53
1:A:96:TYR:CE2	1:A:104:VAL:HG21	2.35	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:O	1:A:216:LEU:CD2	2.57	0.53
1:B:266:LEU:N	1:B:267:PRO:HD2	2.24	0.53
1:A:239:GLU:HB2	1:A:245:LYS:HA	1.91	0.52
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.91	0.52
1:B:102:TYR:CE2	1:B:104:VAL:HA	2.44	0.52
1:B:139:VAL:HG21	1:B:226:LEU:HD23	1.90	0.52
1:A:326:ASN:ND2	1:A:328:LEU:HD11	2.23	0.52
1:A:240:SER:O	1:A:241:ALA:HB2	2.10	0.52
1:B:256:ILE:HG22	1:B:305:ILE:HD13	1.92	0.52
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.92	0.52
10:B:1401:HTO:H72	9:B:1509:HTG:H3'2	1.91	0.52
1:B:245:LYS:HZ1	1:B:248:LYS:HD2	1.74	0.52
1:A:9:PHE:HA	1:A:179:ILE:HD11	1.91	0.52
1:B:216:LEU:O	1:B:220:PHE:HD2	1.92	0.52
1:B:131:LEU:HD23	1:B:254:VAL:HG22	1.92	0.52
1:B:330:ASP:O	1:B:331:ASP:O	2.26	0.52
1:B:71:PRO:O	1:B:74:TYR:HB2	2.11	0.51
1:B:224:GLY:O	1:B:227:VAL:HG12	2.10	0.51
1:B:253:MET:HA	1:B:309:MET:SD	2.50	0.51
1:B:76:LEU:HD22	1:B:306:TYR:CG	2.46	0.51
1:B:143:MET:HG2	1:B:146:PHE:HB2	1.92	0.51
1:B:321:LEU:C	1:B:323:CYS:H	2.14	0.51
1:B:148:PHE:CD1	1:B:152:HIS:HB2	2.46	0.51
1:A:337:VAL:CG2	1:A:338:SER:N	2.72	0.51
1:B:332:GLU:OE1	1:B:332:GLU:O	2.27	0.51
1:B:341:GLU:OE1	1:B:342:THR:HG22	2.10	0.51
1:A:87:VAL:O	1:A:91:PHE:HB2	2.10	0.51
1:B:85:PHE:O	1:B:89:GLY:N	2.40	0.51
1:B:131:LEU:O	1:B:135:ARG:HB2	2.11	0.51
1:A:64:GLN:HE22	1:A:320:THR:HG23	1.74	0.51
1:B:245:LYS:CE	1:B:245:LYS:HA	2.24	0.51
1:A:82:ALA:O	1:A:86:MET:HG3	2.10	0.50
1:B:234:ALA:HA	1:B:245:LYS:HZ3	1.76	0.50
1:B:213:ILE:O	1:B:217:ILE:HG13	2.11	0.50
1:A:180:PRO:HA	1:A:186:SER:O	2.11	0.50
1:A:227:VAL:CG1	1:A:228:PHE:N	2.73	0.50
1:A:65:HIS:ND1	1:A:338:SER:CA	2.73	0.50
1:A:325:LYS:HE2	1:A:327:PRO:CD	2.41	0.50
1:A:337:VAL:C	1:A:338:SER:OG	2.49	0.50
1:A:137:VAL:HA	1:A:142:PRO:CD	2.41	0.50
1:A:225:GLN:C	1:A:227:VAL:H	2.15	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD21	1:B:165:LEU:HD22	1.94	0.50
1:B:238:GLN:CG	1:B:241:ALA:H	2.18	0.50
1:B:340:THR:HG23	1:B:341:GLU:N	2.26	0.50
1:A:74:TYR:OH	1:A:150:GLU:HG2	2.12	0.49
1:A:83:ASP:O	1:A:87:VAL:HG23	2.12	0.49
1:B:236:GLN:O	1:B:237:GLN:C	2.51	0.49
1:B:248:LYS:O	1:B:252:ARG:HG3	2.11	0.49
1:A:134:GLU:HG2	1:A:148:PHE:CE2	2.47	0.49
1:A:239:GLU:CB	1:A:244:GLN:OE1	2.60	0.49
1:A:94:THR:HB	1:A:113:GLU:OE2	2.12	0.49
1:B:240:SER:O	1:B:241:ALA:CB	2.60	0.49
1:A:237:GLN:O	1:A:238:GLN:HB3	2.13	0.49
1:B:96:TYR:CD2	1:B:105:PHE:CE2	3.00	0.49
1:A:238:GLN:HA	1:A:242:THR:N	2.28	0.49
1:B:115:PHE:CD1	1:B:172:LEU:HD11	2.48	0.49
1:B:238:GLN:HG3	1:B:241:ALA:CA	2.42	0.49
1:B:75:ILE:HG13	1:B:131:LEU:HD12	1.93	0.49
1:B:67:LYS:HE3	1:B:312:GLN:OE1	2.13	0.49
1:A:138:VAL:HG23	1:A:139:VAL:N	2.26	0.49
1:B:126:TRP:CD1	1:B:163:MET:HB2	2.46	0.49
1:B:298:SER:HA	1:B:301:TYR:CD2	2.47	0.49
1:A:223:TYR:C	1:A:225:GLN:H	2.16	0.49
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.27	0.49
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.10	0.48
1:B:319:THR:HG22	1:B:341:GLU:OE2	2.13	0.48
1:A:139:VAL:HG21	1:A:230:VAL:HG11	1.94	0.48
1:A:23:PRO:HA	1:A:28:GLN:NE2	2.28	0.48
1:A:322:CYS:HA	8:A:1322:PLM:O2	2.13	0.48
1:B:9:PHE:C	1:B:179:ILE:HD11	2.33	0.48
1:A:245:LYS:O	1:A:245:LYS:NZ	2.41	0.48
1:A:297:THR:O	1:A:300:VAL:HG22	2.13	0.48
1:B:151:ASN:O	1:B:155:MET:HG2	2.14	0.48
1:A:329:GLY:CA	1:B:96:TYR:HE1	2.20	0.48
1:A:327:PRO:O	1:A:328:LEU:C	2.52	0.48
1:B:167:CYS:SG	1:B:211:HIS:CD2	3.07	0.48
1:A:67:LYS:H	1:A:337:VAL:HG23	1.77	0.48
1:B:6:GLY:HA3	1:B:9:PHE:CZ	2.49	0.48
1:A:195:HIS:HD1	1:A:198:THR:CG2	2.27	0.48
1:A:36:GLN:O	1:A:39:MET:HB2	2.13	0.48
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.44	0.47
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HD12	1:B:154:ILE:N	2.28	0.47
1:A:75:ILE:HG21	1:A:131:LEU:CD1	2.43	0.47
1:A:308:MET:CE	1:B:41:ALA:HB1	2.44	0.47
1:A:342:THR:C	1:A:344:GLN:H	2.18	0.47
1:A:85:PHE:O	1:A:89:GLY:N	2.47	0.47
1:A:298:SER:HA	1:A:301:TYR:CE2	2.49	0.47
1:A:332:GLU:C	1:A:334:SER:N	2.60	0.47
1:A:329:GLY:HA2	1:B:96:TYR:CZ	2.46	0.47
3:D:1:NAG:C6	3:D:2:NAG:H82	2.44	0.47
1:B:241:ALA:CB	1:B:243:THR:HG22	2.44	0.47
1:B:338:SER:O	1:B:343:SER:HB2	2.14	0.47
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.96	0.47
1:B:136:TYR:HB2	1:B:222:CYS:SG	2.55	0.47
1:B:75:ILE:HG21	1:B:131:LEU:HD11	1.97	0.47
1:A:314:ARG:O	1:A:318:VAL:HG23	2.15	0.47
1:A:231:LYS:NZ	1:A:233:ALA:HB3	2.30	0.46
1:B:298:SER:HB2	11:B:2036:HOH:O	2.15	0.46
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.15	0.46
1:B:150:GLU:O	1:B:154:ILE:HD13	2.16	0.46
1:A:151:ASN:O	1:A:155:MET:HG2	2.15	0.46
1:A:158:ALA:O	1:A:162:VAL:HG23	2.15	0.46
1:B:68:LEU:HA	1:B:73:ASN:ND2	2.31	0.46
1:B:302:ASN:HB2	11:B:2016:HOH:O	2.16	0.46
1:B:64:GLN:NE2	1:B:320:THR:OG1	2.49	0.46
1:A:241:ALA:C	1:A:243:THR:N	2.68	0.46
1:A:319:THR:OG1	1:A:327:PRO:HB3	2.16	0.46
1:B:139:VAL:HB	1:B:226:LEU:HG	1.97	0.46
1:B:198:THR:CG2	1:B:200:ASN:OD1	2.64	0.45
1:A:223:TYR:C	1:A:225:GLN:N	2.68	0.45
1:B:171:PRO:HG2	1:B:189:ILE:HD11	1.98	0.45
1:B:226:LEU:CD1	1:B:226:LEU:N	2.80	0.45
1:B:96:TYR:HE2	1:B:104:VAL:HG21	1.80	0.45
1:B:227:VAL:CG1	1:B:228:PHE:N	2.80	0.45
1:A:134:GLU:HG2	1:A:148:PHE:CD2	2.52	0.45
1:A:338:SER:OG	1:A:341:GLU:OE2	2.33	0.45
1:A:67:LYS:H	1:A:337:VAL:HG21	1.82	0.45
1:A:308:MET:HE1	1:B:99:LEU:HD21	1.98	0.45
1:A:194:PRO:O	1:A:195:HIS:C	2.55	0.45
1:A:266:LEU:N	1:A:267:PRO:HD2	2.31	0.45
1:B:328:LEU:O	1:B:329:GLY:C	2.55	0.45
1:B:332:GLU:CB	1:B:336:THR:HG22	2.46	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:HA	1:A:242:THR:HA	1.99	0.45
1:A:311:LYS:HZ1	1:A:330:ASP:HB2	1.80	0.45
1:B:198:THR:HG23	1:B:200:ASN:OD1	2.17	0.45
1:B:67:LYS:HE2	1:B:316:CYS:SG	2.56	0.45
1:A:24:PHE:CD1	1:A:106:GLY:HA2	2.51	0.45
1:A:66:LYS:N	1:A:66:LYS:HD2	2.32	0.45
1:B:64:GLN:HE21	1:B:65:HIS:CD2	2.34	0.45
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.78	0.45
1:B:107:PRO:O	1:B:111:ASN:ND2	2.50	0.45
1:B:66:LYS:HD3	1:B:343:SER:OG	2.16	0.45
1:A:143:MET:HB2	1:A:146:PHE:HB3	1.99	0.45
1:A:169:ALA:N	1:A:170:PRO:CD	2.80	0.44
1:B:67:LYS:NZ	1:B:335:THR:O	2.50	0.44
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.83	0.44
1:A:70:THR:O	1:A:74:TYR:HD2	1.98	0.44
1:B:236:GLN:O	1:B:238:GLN:O	2.36	0.44
1:B:227:VAL:HG13	1:B:228:PHE:N	2.32	0.44
1:A:135:ARG:HE	1:A:135:ARG:HA	1.80	0.44
1:B:240:SER:O	1:B:241:ALA:HB2	2.18	0.44
1:A:332:GLU:O	1:A:332:GLU:OE1	2.35	0.44
1:B:243:THR:HG23	1:B:244:GLN:N	2.32	0.44
1:B:39:MET:HA	1:B:39:MET:CE	2.48	0.44
1:A:67:LYS:HB2	1:A:337:VAL:CG2	2.48	0.44
1:B:150:GLU:O	1:B:154:ILE:CD1	2.65	0.44
1:B:140:CYS:O	1:B:141:LYS:C	2.56	0.44
1:A:137:VAL:HA	1:A:142:PRO:HD3	1.99	0.44
1:A:135:ARG:NH2	1:A:138:VAL:HG21	2.33	0.43
1:A:239:GLU:CB	1:A:244:GLN:NE2	2.81	0.43
1:B:189:ILE:HA	1:B:189:ILE:HD13	1.87	0.43
1:B:196:GLU:C	1:B:198:THR:N	2.71	0.43
1:B:230:VAL:O	1:B:230:VAL:HG13	2.17	0.43
1:B:64:GLN:HE22	1:B:320:THR:HG23	1.83	0.43
1:A:227:VAL:CG1	1:A:228:PHE:H	2.31	0.43
1:A:326:ASN:ND2	1:A:328:LEU:HD21	2.33	0.43
1:B:195:HIS:HD1	1:B:198:THR:HG22	1.81	0.43
1:B:230:VAL:HB	1:B:248:LYS:NZ	2.33	0.43
1:A:346:ALA:N	1:A:347:PRO:HD3	2.33	0.43
1:A:224:GLY:O	1:A:227:VAL:HG12	2.18	0.43
1:B:332:GLU:OE2	1:B:334:SER:HB2	2.18	0.43
1:B:79:LEU:CD1	1:B:79:LEU:N	2.81	0.43
1:A:236:GLN:O	1:A:245:LYS:HD2	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD13	1:A:77:LEU:HD11	2.00	0.43
1:B:135:ARG:O	1:B:226:LEU:HD21	2.18	0.43
1:B:256:ILE:HD13	1:B:256:ILE:HA	1.73	0.43
1:A:131:LEU:O	1:A:135:ARG:HB2	2.19	0.43
1:A:231:LYS:HZ2	1:A:233:ALA:HB3	1.84	0.43
1:B:65:HIS:HA	1:B:338:SER:C	2.39	0.43
1:B:9:PHE:HA	1:B:179:ILE:CG1	2.48	0.43
1:A:133:ILE:O	1:A:136:TYR:N	2.52	0.43
1:A:239:GLU:HG2	1:A:248:LYS:HZ1	1.83	0.43
1:B:239:GLU:OE1	1:B:239:GLU:HA	2.18	0.43
1:B:79:LEU:CD1	1:B:79:LEU:H	2.32	0.43
1:A:178:TYR:HA	1:A:188:GLY:O	2.19	0.43
1:A:74:TYR:CZ	1:A:150:GLU:HG2	2.53	0.43
1:A:77:LEU:O	1:A:81:VAL:HG23	2.18	0.43
1:B:221:PHE:CD1	1:B:221:PHE:C	2.91	0.43
1:B:243:THR:CG2	1:B:244:GLN:N	2.82	0.43
1:A:129:VAL:O	1:A:133:ILE:HG12	2.17	0.43
1:A:175:TRP:O	1:A:176:SER:HB3	2.19	0.43
1:A:72:LEU:HD21	1:A:253:MET:HE1	2.01	0.43
1:B:75:ILE:HG23	1:B:127:SER:HB3	2.00	0.43
1:A:321:LEU:O	1:A:323:CYS:N	2.49	0.42
1:B:67:LYS:HZ2	1:B:332:GLU:HG3	1.84	0.42
1:A:321:LEU:C	1:A:323:CYS:N	2.72	0.42
1:B:134:GLU:O	1:B:138:VAL:HG13	2.19	0.42
1:B:42:ALA:HB2	9:B:1508:HTG:H7'3	2.01	0.42
1:B:236:GLN:O	1:B:238:GLN:N	2.52	0.42
1:B:204:VAL:HG11	1:B:276:PHE:CD1	2.55	0.42
1:B:210:VAL:HA	1:B:214:ILE:HD12	2.01	0.42
1:A:326:ASN:OD1	1:A:328:LEU:HD13	2.20	0.42
1:B:139:VAL:CG1	1:B:226:LEU:HG	2.49	0.42
1:A:175:TRP:CD2	1:A:203:PHE:HD1	2.38	0.42
1:A:42:ALA:O	1:A:45:PHE:HB3	2.19	0.42
1:B:312:GLN:O	1:B:316:CYS:SG	2.78	0.42
1:B:67:LYS:NZ	1:B:336:THR:HA	2.35	0.42
1:B:196:GLU:C	1:B:198:THR:H	2.23	0.42
1:B:137:VAL:HG12	1:B:137:VAL:O	2.20	0.42
1:B:330:ASP:C	1:B:331:ASP:O	2.58	0.42
1:B:99:LEU:HA	1:B:99:LEU:HD23	1.92	0.42
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.55	0.41
1:B:290:ILE:HB	1:B:291:PRO:CD	2.50	0.41
1:A:136:TYR:HA	1:A:226:LEU:HD11	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:O	1:A:212:PHE:HB2	2.20	0.41
1:A:213:ILE:O	1:A:217:ILE:HG13	2.20	0.41
1:B:245:LYS:HG3	1:B:245:LYS:O	2.18	0.41
1:B:249:GLU:HG3	1:B:250:VAL:N	2.35	0.41
1:B:338:SER:OG	1:B:341:GLU:CD	2.58	0.41
7:A:1296:RET:H8	7:A:1296:RET:H181	2.02	0.41
1:A:75:ILE:HG13	1:A:131:LEU:HD11	2.01	0.41
1:B:208:PHE:O	1:B:213:ILE:CG1	2.65	0.41
1:B:238:GLN:HG3	1:B:241:ALA:C	2.41	0.41
1:B:71:PRO:O	1:B:74:TYR:N	2.52	0.41
1:A:314:ARG:HD2	1:B:99:LEU:HD13	2.02	0.41
1:A:75:ILE:HA	1:A:75:ILE:HD13	1.79	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.89	0.41
1:B:146:PHE:CE1	1:B:152:HIS:NE2	2.89	0.41
1:B:253:MET:HE1	1:B:306:TYR:CD1	2.55	0.41
1:B:33:GLU:HB2	1:B:36:GLN:HG3	2.03	0.41
1:B:60:TYR:C	1:B:60:TYR:CD1	2.93	0.41
1:A:135:ARG:O	1:A:138:VAL:HG22	2.20	0.41
1:A:229:THR:HG22	1:A:230:VAL:H	1.86	0.41
1:B:67:LYS:HE3	1:B:312:GLN:CG	2.51	0.41
1:A:216:LEU:HD12	1:A:220:PHE:CE2	2.56	0.41
1:A:332:GLU:O	1:A:334:SER:N	2.49	0.41
1:B:87:VAL:O	1:B:91:PHE:HB2	2.20	0.41
1:A:155:MET:HA	1:A:155:MET:CE	2.51	0.41
1:A:244:GLN:O	1:A:244:GLN:OE1	2.38	0.41
1:A:239:GLU:CG	1:A:248:LYS:HZ2	2.31	0.41
1:A:326:ASN:C	1:A:328:LEU:H	2.23	0.41
1:B:231:LYS:HZ1	1:B:233:ALA:HB3	1.83	0.41
1:A:126:TRP:CE2	1:A:163:MET:HB3	2.55	0.41
1:B:241:ALA:HB3	1:B:243:THR:HG22	2.03	0.41
1:B:68:LEU:C	1:B:69:ARG:HG2	2.41	0.41
1:A:11:VAL:CG1	1:A:31:LEU:HD21	2.51	0.41
1:B:216:LEU:HD13	1:B:216:LEU:HA	1.83	0.41
1:A:259:ILE:O	1:A:263:ILE:HG13	2.20	0.41
1:B:175:TRP:O	1:B:176:SER:HB3	2.20	0.41
1:B:65:HIS:CB	1:B:338:SER:HA	2.51	0.41
1:A:176:SER:OG	1:A:177:ARG:N	2.53	0.40
1:A:248:LYS:HE3	1:A:248:LYS:HB2	1.80	0.40
1:A:182:GLY:HA2	1:A:285:PRO:O	2.21	0.40
1:B:67:LYS:CB	1:B:337:VAL:CG2	2.99	0.40
1:A:347:PRO:HB2	1:A:348:ALA:H	1.48	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:HG21	1:B:156:GLY:O	2.20	0.40
1:B:205:ILE:O	1:B:209:VAL:HG23	2.21	0.40
1:A:240:SER:O	1:A:241:ALA:CB	2.68	0.40
1:B:128:LEU:HD22	1:B:258:VAL:HG22	2.04	0.40
1:B:96:TYR:HE2	1:B:104:VAL:HG22	1.86	0.40
1:A:208:PHE:O	1:A:213:ILE:HG13	2.21	0.40
1:A:298:SER:HB2	11:A:2015:HOH:O	2.21	0.40
1:A:332:GLU:O	1:A:333:ALA:HB3	2.21	0.40
1:A:85:PHE:O	1:A:89:GLY:HA3	2.21	0.40
1:B:139:VAL:HG13	1:B:230:VAL:HG12	1.98	0.40
1:B:231:LYS:HE3	1:B:231:LYS:HB2	1.80	0.40
1:B:65:HIS:CE1	1:B:338:SER:OG	2.75	0.40
1:A:326:ASN:ND2	1:A:328:LEU:CD1	2.85	0.40
1:A:97:THR:HG23	1:A:102:TYR:C	2.42	0.40
1:B:136:TYR:CE1	1:B:225:GLN:HG3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	9:B:1509:HTG:O6[4_564]	2.04	0.16

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	347/349 (99%)	293 (84%)	36 (10%)	18 (5%)	2	0
1	B	347/349 (99%)	288 (83%)	43 (12%)	16 (5%)	2	1
All	All	694/698 (99%)	581 (84%)	79 (11%)	34 (5%)	2	1

All (34) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	145	ASN
1	A	195	HIS
1	A	212	PHE
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	328	LEU
1	A	341	GLU
1	A	347	PRO
1	B	237	GLN
1	B	240	SER
1	B	241	ALA
1	B	331	ASP
1	B	337	VAL
1	A	329	GLY
1	A	335	THR
1	B	195	HIS
1	B	229	THR
1	B	238	GLN
1	B	323	CYS
1	B	347	PRO
1	A	322	CYS
1	A	338	SER
1	B	235	ALA
1	B	328	LEU
1	B	341	GLU
1	A	229	THR
1	A	238	GLN
1	B	141	LYS
1	A	141	LYS
1	B	334	SER
1	B	324	GLY
1	A	139	VAL
1	A	324	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	296/296 (100%)	275 (93%)	21 (7%)	14	16
1	B	296/296 (100%)	275 (93%)	21 (7%)	14	16
All	All	592/592 (100%)	550 (93%)	42 (7%)	14	16

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	57	LEU
1	A	76	LEU
1	A	79	LEU
1	A	94	THR
1	A	119	LEU
1	A	134	GLU
1	A	135	ARG
1	A	143	MET
1	A	216	LEU
1	A	237	GLN
1	A	239	GLU
1	A	244	GLN
1	A	245	LYS
1	A	252	ARG
1	A	266	LEU
1	A	331	ASP
1	A	332	GLU
1	A	336	THR
1	A	337	VAL
1	A	343	SER
1	B	8	ASN
1	B	38	SER
1	B	50	LEU
1	B	94	THR
1	B	119	LEU
1	B	134	GLU
1	B	135	ARG
1	B	143	MET
1	B	148	PHE
1	B	167	CYS
1	B	222	CYS
1	B	229	THR
1	B	231	LYS
1	B	236	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	237	GLN
1	B	244	GLN
1	B	245	LYS
1	B	249	GLU
1	B	264	CYS
1	B	330	ASP
1	B	332	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	64	GLN
1	A	73	ASN
1	A	100	HIS
1	A	111	ASN
1	A	225	GLN
1	A	237	GLN
1	A	326	ASN
1	B	8	ASN
1	B	64	GLN
1	B	73	ASN
1	B	100	HIS
1	B	111	ASN
1	B	151	ASN
1	B	237	GLN
1	B	244	GLN
1	B	302	ASN

### 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 ⓘ

11 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	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.84	0
2	NAG	C	2	2	14,14,15	0.76	0	17,19,21	0.90	1 (5%)
2	MAN	C	3	2	11,11,12	0.92	0	15,15,17	0.84	0
3	NAG	D	1	1,3	14,14,15	0.62	0	17,19,21	0.67	0
3	NAG	D	2	3	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.44	0	17,19,21	0.70	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
4	BMA	E	3	4	11,11,12	0.74	0	15,15,17	0.65	0
4	BMA	E	4	4	11,11,12	0.91	1 (9%)	15,15,17	0.95	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.56	0	17,19,21	0.78	0
3	NAG	F	2	3	14,14,15	0.68	0	17,19,21	0.76	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	BMA	C2-C3	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C2-N2-C7	-3.29	118.22	122.90
3	D	2	NAG	C2-N2-C7	-2.71	119.05	122.90
4	E	4	BMA	C1-O5-C5	2.37	115.41	112.19
2	C	2	NAG	C8-C7-N2	2.11	119.67	116.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

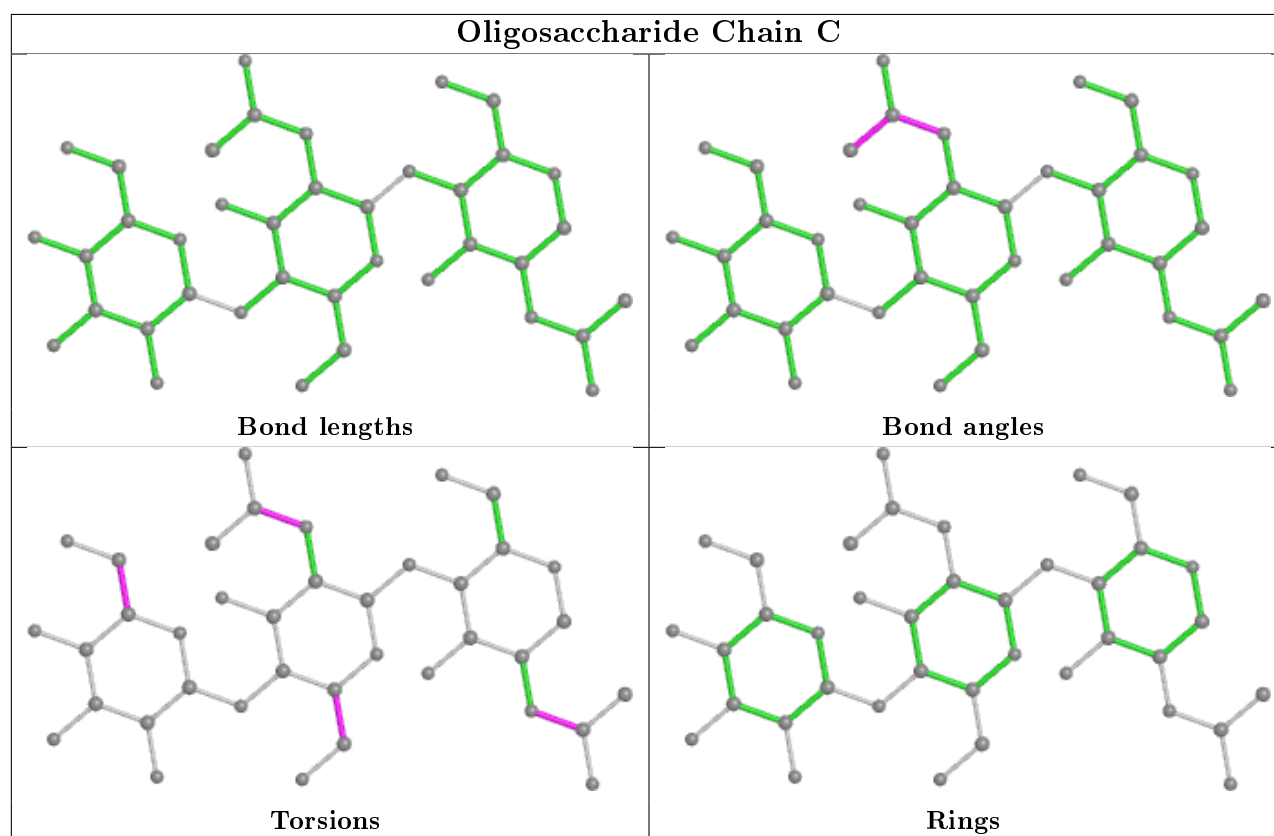
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

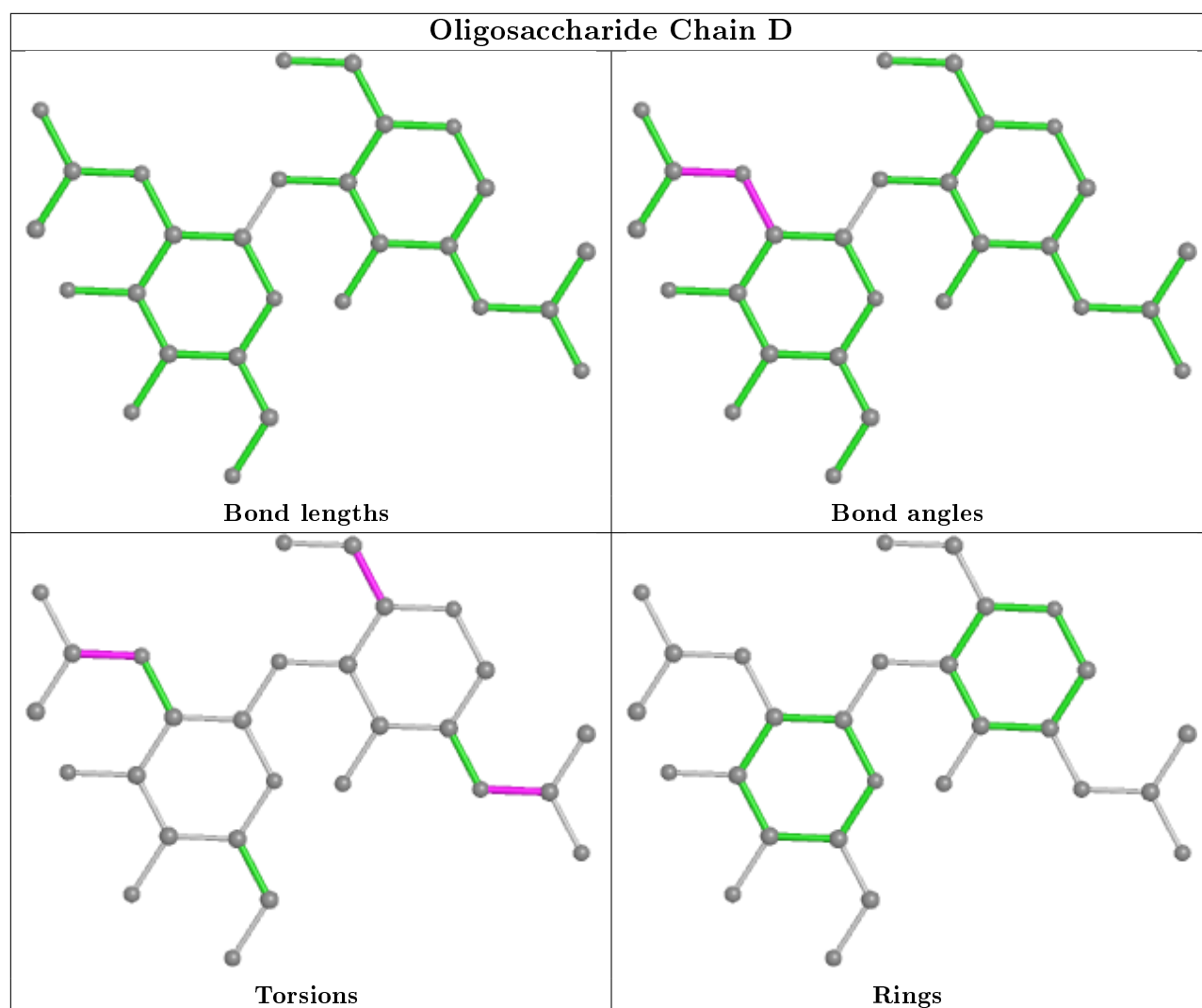
There are no ring outliers.

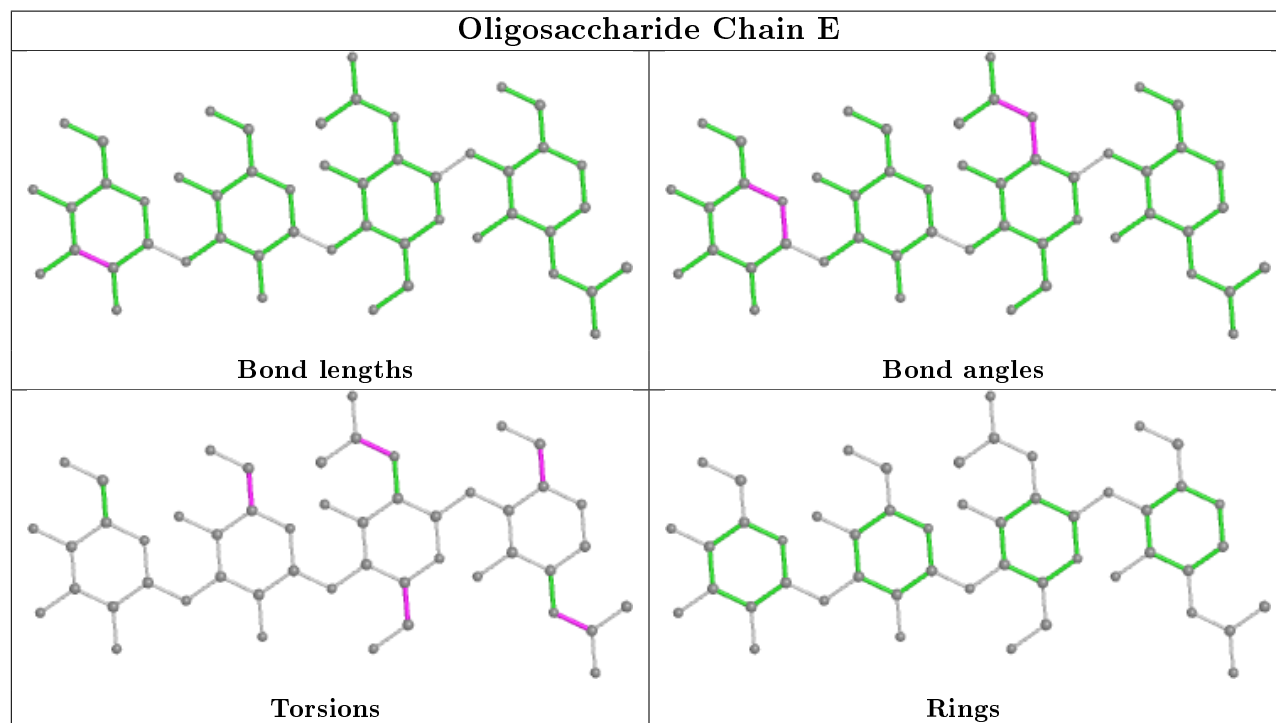
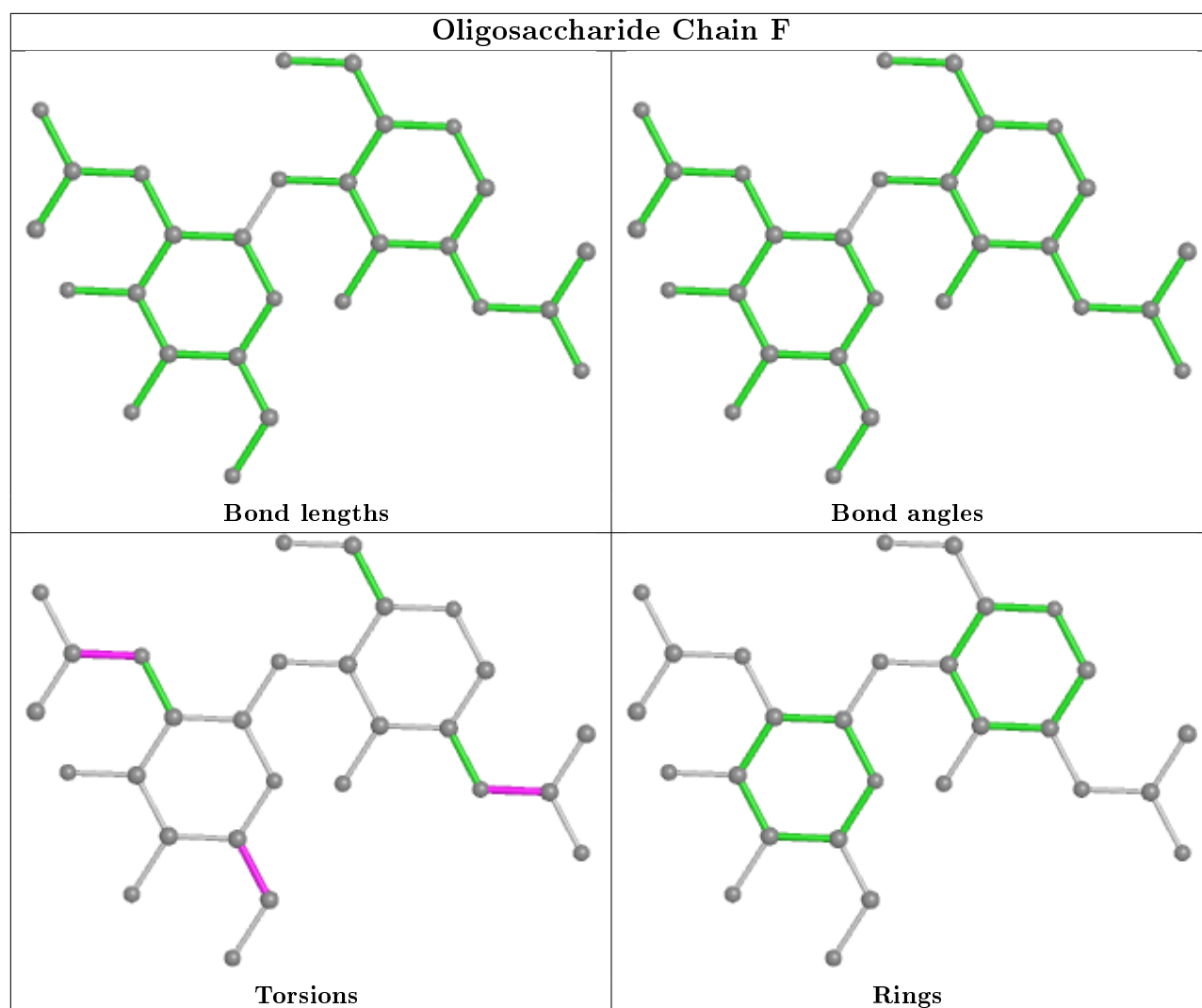
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	2	0
3	D	1	NAG	2	0
2	C	2	NAG	1	0
2	C	1	NAG	1	0

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









## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PLM	B	1323	1	16,16,17	0.49	0	15,15,17	0.49	0
7	RET	B	1296	1	20,20,21	2.47	4 (20%)	27,27,28	1.67	8 (29%)
8	PLM	A	1410	-	15,15,17	1.88	3 (20%)	14,14,17	3.38	6 (42%)
10	HTO	B	1401	-	9,9,9	1.73	1 (11%)	10,10,10	1.12	1 (10%)
9	HTG	B	1509	-	19,19,19	3.07	8 (42%)	23,24,24	2.37	2 (8%)
9	HTG	A	1507	-	19,19,19	3.18	8 (42%)	23,24,24	2.31	2 (8%)
8	PLM	A	1322	1	16,16,17	0.29	0	15,15,17	0.70	0
8	PLM	B	1322	1	16,16,17	0.49	0	15,15,17	0.47	0
9	HTG	B	1508	-	19,19,19	2.45	7 (36%)	23,24,24	2.53	2 (8%)
8	PLM	B	1407	-	15,15,17	1.75	3 (20%)	14,14,17	3.38	7 (50%)
9	HTG	B	1506	-	19,19,19	3.24	8 (42%)	23,24,24	1.95	2 (8%)
7	RET	A	1296	1	20,20,21	1.95	3 (15%)	27,27,28	1.78	8 (29%)
8	PLM	A	1323	1	16,16,17	0.38	0	15,15,17	0.55	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
8	PLM	B	1323	1	-	8/13/14/15	-
7	RET	B	1296	1	-	1/13/30/31	0/1/1/1
8	PLM	A	1410	-	-	5/13/13/15	-
10	HTO	B	1401	-	-	1/10/10/10	-
9	HTG	B	1509	-	-	4/10/30/30	0/1/1/1
9	HTG	A	1507	-	-	4/10/30/30	0/1/1/1
8	PLM	A	1322	1	-	10/13/14/15	-
8	PLM	B	1322	1	-	10/13/14/15	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTG	B	1508	-	-	4/10/30/30	0/1/1/1
8	PLM	B	1407	-	-	6/13/13/15	-
9	HTG	B	1506	-	-	2/10/30/30	0/1/1/1
7	RET	A	1296	1	-	1/13/30/31	0/1/1/1
8	PLM	A	1323	1	-	9/13/14/15	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1506	HTG	O5-C1	9.62	1.57	1.42
9	A	1507	HTG	O5-C1	9.16	1.56	1.42
9	B	1509	HTG	O5-C1	8.32	1.55	1.42
9	B	1508	HTG	O5-C1	6.96	1.53	1.42
7	B	1296	RET	C1-C6	5.76	1.61	1.53
7	B	1296	RET	C5-C6	5.63	1.44	1.34
7	B	1296	RET	C14-C13	5.51	1.38	1.33
9	B	1509	HTG	C4-C5	5.21	1.64	1.53
9	A	1507	HTG	C1-S1	5.20	1.88	1.80
9	B	1509	HTG	C1-C2	5.05	1.62	1.53
7	A	1296	RET	C5-C6	5.05	1.43	1.34
8	A	1410	PLM	CC-CB	-4.95	1.23	1.51
9	A	1507	HTG	C1-C2	4.77	1.61	1.53
9	B	1506	HTG	C1-S1	4.60	1.87	1.80
8	B	1407	PLM	CC-CB	-4.59	1.25	1.51
7	A	1296	RET	C1-C6	4.57	1.60	1.53
10	B	1401	HTO	C3-C2	4.22	1.63	1.52
9	B	1506	HTG	C4-C5	4.16	1.61	1.53
9	B	1506	HTG	C1-C2	3.85	1.60	1.53
9	B	1509	HTG	O5-C5	3.72	1.53	1.44
9	B	1508	HTG	C4-C5	3.64	1.60	1.53
9	B	1509	HTG	C1-S1	3.62	1.86	1.80
9	B	1506	HTG	C4-C3	3.61	1.61	1.52
8	A	1410	PLM	CB-CA	-3.56	1.31	1.51
9	B	1506	HTG	C1'-S1	3.53	1.86	1.81
9	A	1507	HTG	C1'-S1	3.49	1.86	1.81
9	B	1506	HTG	C3-C2	3.44	1.61	1.52
9	B	1508	HTG	O5-C5	3.41	1.52	1.44
9	A	1507	HTG	C4-C3	3.41	1.61	1.52
9	B	1506	HTG	O5-C5	3.36	1.52	1.44
9	B	1509	HTG	C4-C3	3.35	1.60	1.52
9	A	1507	HTG	C3-C2	3.35	1.60	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1508	HTG	C1-C2	3.26	1.59	1.53
8	B	1407	PLM	CB-CA	-3.23	1.33	1.51
9	A	1507	HTG	C4-C5	3.18	1.59	1.53
8	A	1410	PLM	CD-CC	-3.07	1.34	1.51
9	B	1509	HTG	C3-C2	3.07	1.60	1.52
9	B	1508	HTG	C3-C2	3.02	1.60	1.52
9	A	1507	HTG	O5-C5	2.94	1.51	1.44
9	B	1508	HTG	C4-C3	2.80	1.59	1.52
9	B	1509	HTG	C6-C5	2.73	1.61	1.51
8	B	1407	PLM	CD-CC	-2.66	1.36	1.51
7	A	1296	RET	C14-C13	2.56	1.35	1.33
9	B	1508	HTG	C1-S1	2.12	1.84	1.80
7	B	1296	RET	C17-C1	2.11	1.57	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1508	HTG	C1'-S1-C1	11.32	121.26	100.09
9	B	1509	HTG	C1'-S1-C1	10.42	119.58	100.09
9	A	1507	HTG	C1'-S1-C1	10.07	118.93	100.09
9	B	1506	HTG	C1'-S1-C1	8.43	115.86	100.09
8	B	1407	PLM	CD-CC-CB	8.25	156.30	114.42
8	A	1410	PLM	CD-CC-CB	8.15	155.82	114.42
8	A	1410	PLM	CA-C9-C8	7.53	152.67	114.42
8	B	1407	PLM	CA-C9-C8	7.35	151.72	114.42
7	A	1296	RET	C18-C5-C6	3.90	128.91	124.53
7	B	1296	RET	C18-C5-C6	3.38	128.32	124.53
7	A	1296	RET	C20-C13-C12	3.35	123.36	118.08
7	A	1296	RET	C7-C8-C9	3.31	131.23	126.23
8	B	1407	PLM	CC-CB-CA	3.31	131.22	114.42
8	A	1410	PLM	CC-CB-CA	3.22	130.76	114.42
7	B	1296	RET	C20-C13-C12	3.06	122.90	118.08
7	B	1296	RET	C7-C8-C9	2.85	130.54	126.23
7	A	1296	RET	C19-C9-C10	2.70	126.71	122.92
8	B	1407	PLM	CE-CD-CC	2.60	127.62	114.42
7	B	1296	RET	C19-C9-C10	2.55	126.50	122.92
8	A	1410	PLM	C5-C4-C3	2.53	127.24	114.42
7	B	1296	RET	C8-C9-C10	-2.51	115.08	118.94
7	A	1296	RET	C2-C1-C6	2.46	114.27	110.48
8	A	1410	PLM	CE-CD-CC	2.43	126.77	114.42
9	B	1509	HTG	C2'-C1'-S1	-2.41	104.63	112.40
8	B	1407	PLM	C5-C4-C3	2.37	126.44	114.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1296	RET	C8-C9-C10	-2.32	115.38	118.94
7	A	1296	RET	C18-C5-C4	-2.32	109.16	113.62
7	A	1296	RET	C1-C6-C5	-2.32	119.35	122.61
9	A	1507	HTG	O5-C1-C2	-2.26	107.47	110.31
7	B	1296	RET	C2-C1-C6	2.25	113.94	110.48
10	B	1401	HTO	O3-C3-C4	-2.18	104.41	109.15
8	A	1410	PLM	CF-CE-CD	-2.15	95.35	115.30
9	B	1508	HTG	O5-C5-C6	2.08	111.60	106.44
8	B	1407	PLM	C9-C8-C7	2.08	124.97	114.42
9	B	1506	HTG	O5-C5-C6	2.06	111.56	106.44
8	B	1407	PLM	CF-CE-CD	-2.02	96.57	115.30
7	B	1296	RET	C1-C6-C5	-2.02	119.77	122.61
7	B	1296	RET	C18-C5-C4	-2.01	109.76	113.62

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1296	RET	C10-C11-C12-C13
7	A	1296	RET	C10-C11-C12-C13
8	B	1407	PLM	CA-CB-CC-CD
9	B	1509	HTG	O5-C5-C6-O6
9	A	1507	HTG	O5-C5-C6-O6
9	B	1509	HTG	C4-C5-C6-O6
9	A	1507	HTG	C4-C5-C6-O6
9	B	1506	HTG	C1'-C2'-C3'-C4'
8	B	1322	PLM	C5-C6-C7-C8
8	B	1323	PLM	CA-CB-CC-CD
9	B	1508	HTG	C1'-C2'-C3'-C4'
9	A	1507	HTG	C2'-C3'-C4'-C5'
8	A	1322	PLM	CC-CD-CE-CF
8	A	1410	PLM	CA-CB-CC-CD
8	B	1323	PLM	C3-C4-C5-C6
8	B	1323	PLM	C9-CA-CB-CC
8	A	1323	PLM	CB-CC-CD-CE
8	A	1410	PLM	C5-C6-C7-C8
8	A	1323	PLM	C4-C5-C6-C7
9	B	1509	HTG	C2'-C3'-C4'-C5'
8	A	1323	PLM	C7-C8-C9-CA
8	A	1410	PLM	C9-CA-CB-CC
8	B	1323	PLM	C8-C9-CA-CB
9	B	1508	HTG	C2'-C3'-C4'-C5'

*Continued on next page...*

*Continued from previous page...*

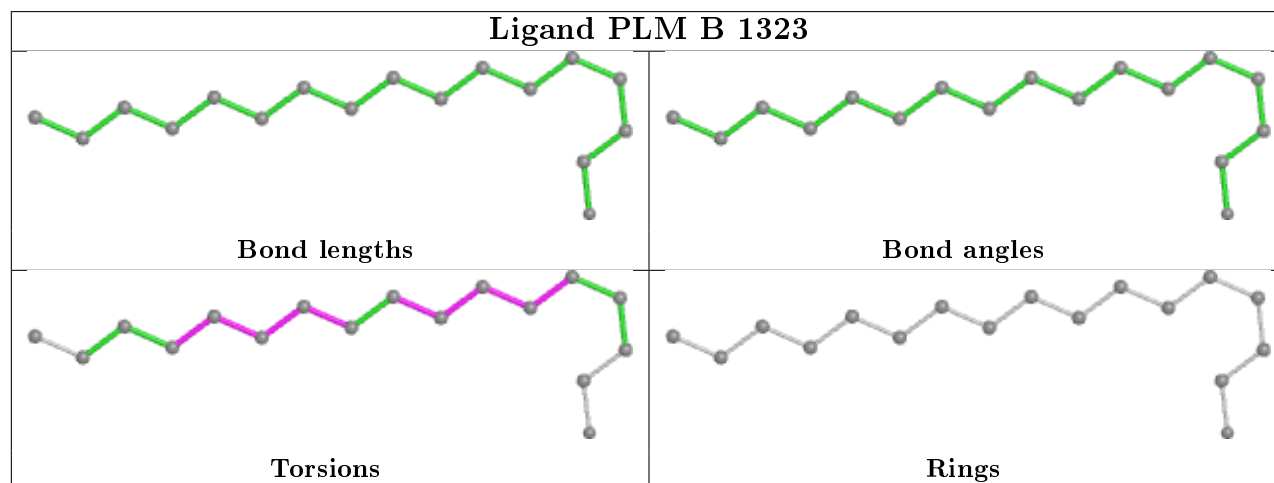
Mol	Chain	Res	Type	Atoms
8	A	1322	PLM	C8-C9-CA-CB
8	B	1322	PLM	CB-CC-CD-CE
8	A	1322	PLM	C4-C5-C6-C7
8	B	1407	PLM	C5-C6-C7-C8
8	B	1323	PLM	C6-C7-C8-C9
9	B	1506	HTG	C2'-C3'-C4'-C5'
8	B	1322	PLM	C9-CA-CB-CC
8	A	1322	PLM	CB-CC-CD-CE
8	B	1322	PLM	CC-CD-CE-CF
9	B	1509	HTG	C3'-C4'-C5'-C6'
8	B	1322	PLM	C8-C9-CA-CB
8	B	1323	PLM	CB-CC-CD-CE
8	A	1322	PLM	C7-C8-C9-CA
8	A	1322	PLM	C9-CA-CB-CC
8	B	1323	PLM	C4-C5-C6-C7
8	A	1410	PLM	C7-C8-C9-CA
10	B	1401	HTO	C4-C5-C6-C7
8	A	1323	PLM	CA-CB-CC-CD
9	B	1508	HTG	C4'-C5'-C6'-C7'
8	A	1322	PLM	C5-C6-C7-C8
8	A	1323	PLM	C2-C3-C4-C5
8	A	1322	PLM	C2-C3-C4-C5
8	A	1323	PLM	C3-C4-C5-C6
8	B	1323	PLM	C5-C6-C7-C8
8	A	1322	PLM	C3-C4-C5-C6
8	B	1407	PLM	C2-C3-C4-C5
8	B	1407	PLM	C3-C4-C5-C6
8	A	1322	PLM	C1-C2-C3-C4
8	B	1322	PLM	C1-C2-C3-C4
8	A	1323	PLM	C1-C2-C3-C4
8	B	1407	PLM	C7-C8-C9-CA
8	B	1322	PLM	C3-C4-C5-C6
8	B	1322	PLM	C4-C5-C6-C7
8	B	1322	PLM	CA-CB-CC-CD
8	A	1323	PLM	C6-C7-C8-C9
8	B	1322	PLM	C7-C8-C9-CA
9	B	1508	HTG	C3'-C4'-C5'-C6'
8	B	1407	PLM	C9-CA-CB-CC
9	A	1507	HTG	C4'-C5'-C6'-C7'
8	A	1410	PLM	CC-CD-CE-CF
8	A	1323	PLM	C8-C9-CA-CB

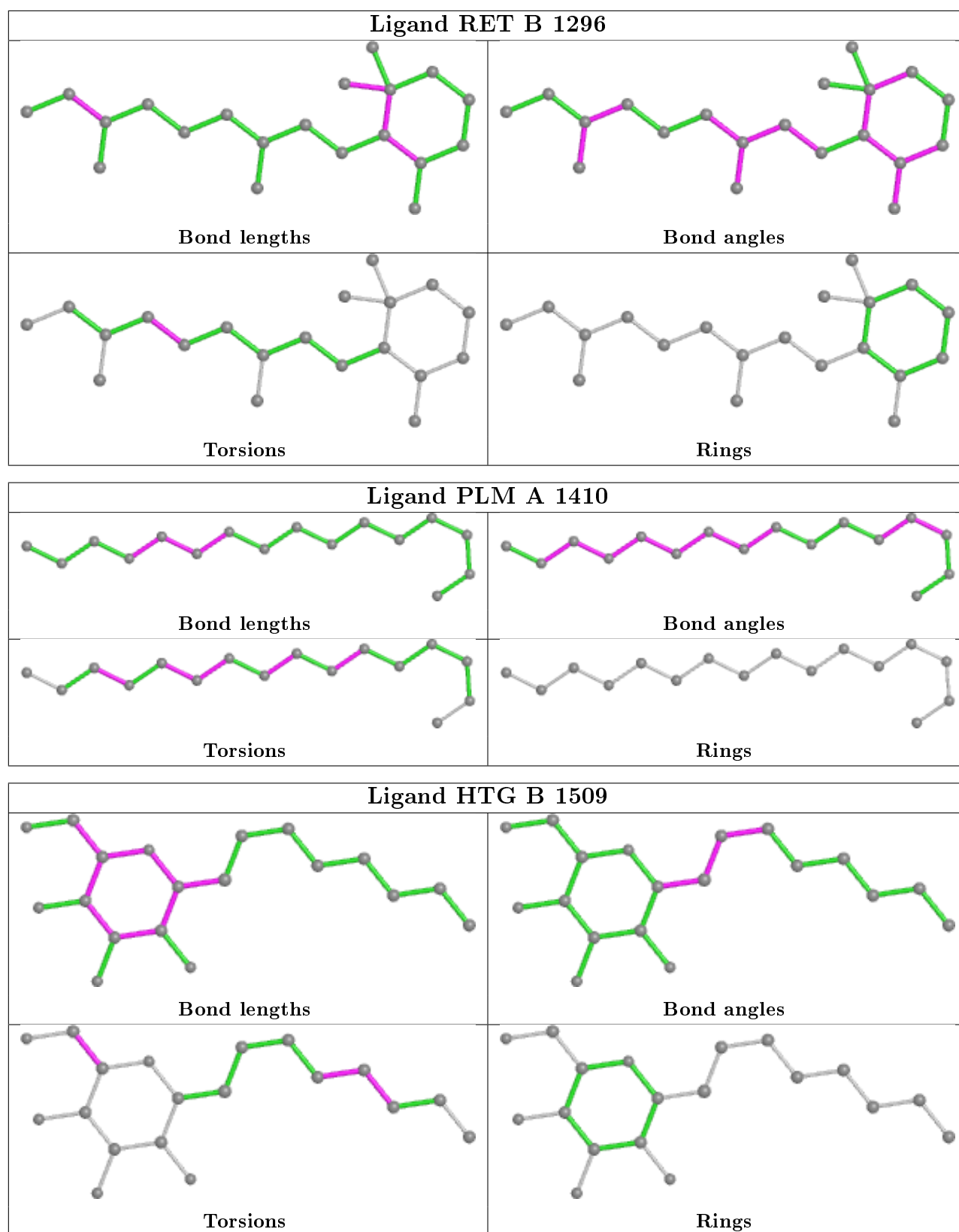
There are no ring outliers.

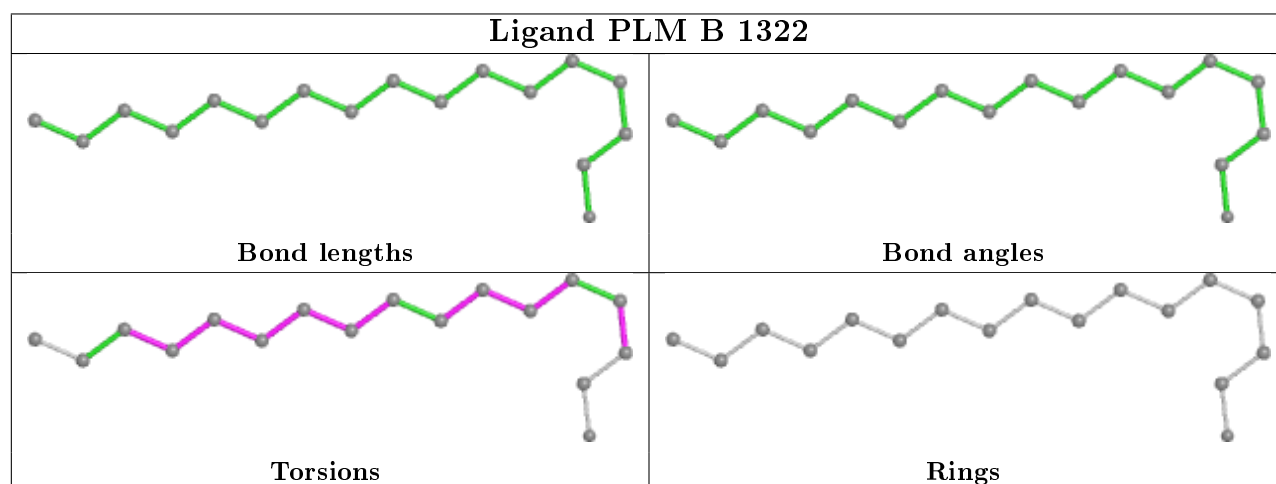
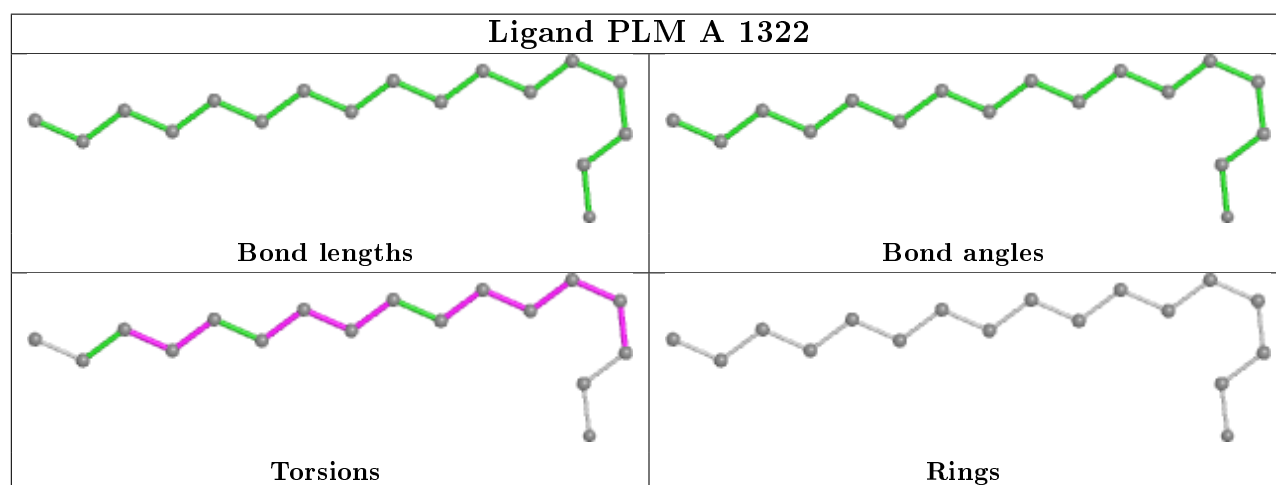
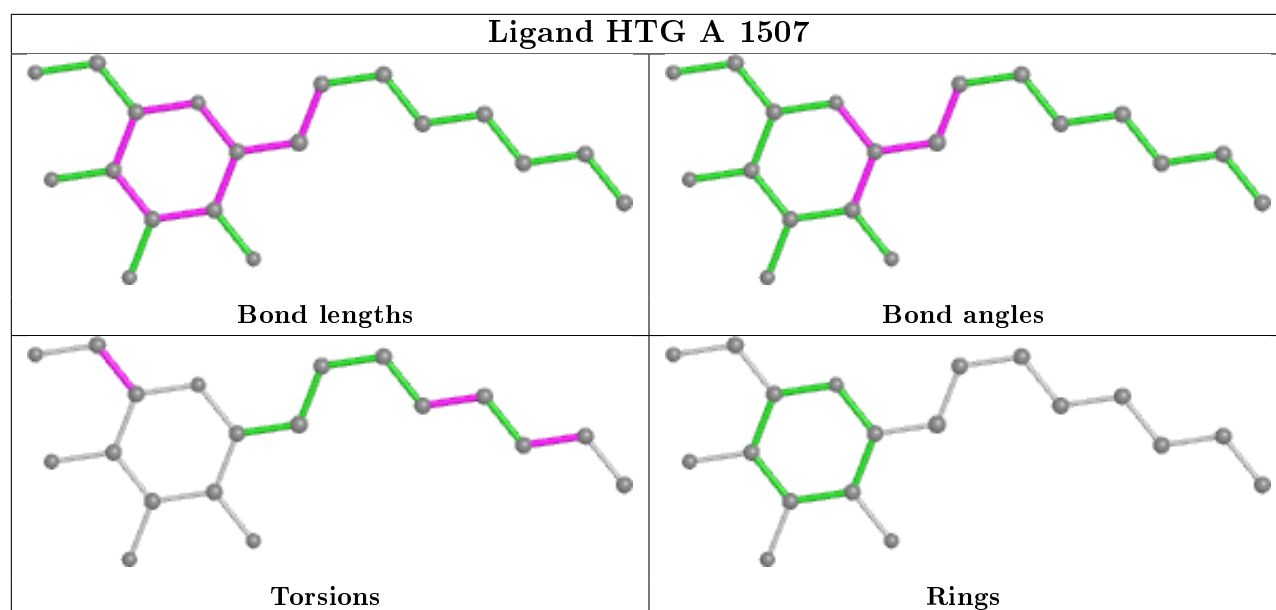
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1323	PLM	3	0
8	A	1410	PLM	1	0
10	B	1401	HTO	1	0
9	B	1509	HTG	1	1
8	A	1322	PLM	3	0
8	B	1322	PLM	2	0
9	B	1508	HTG	2	0
8	B	1407	PLM	1	0
7	A	1296	RET	1	0

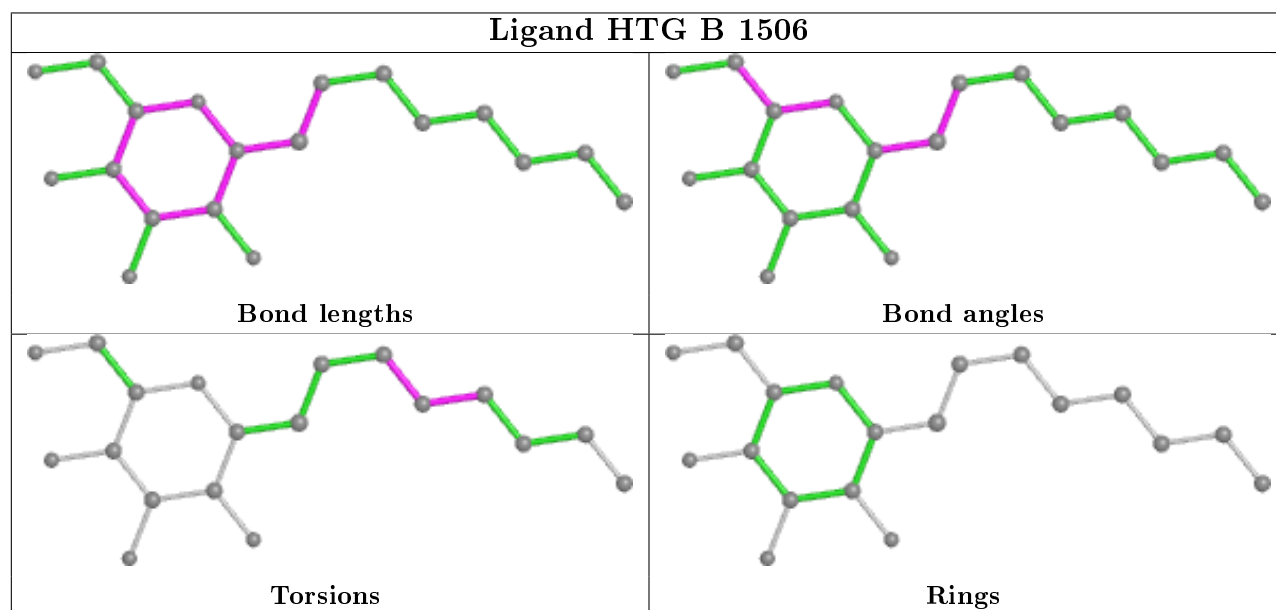
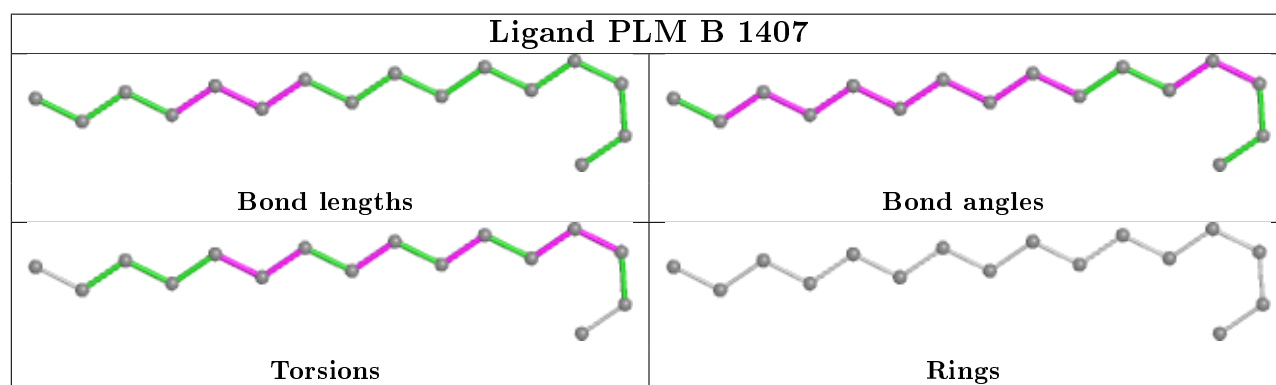
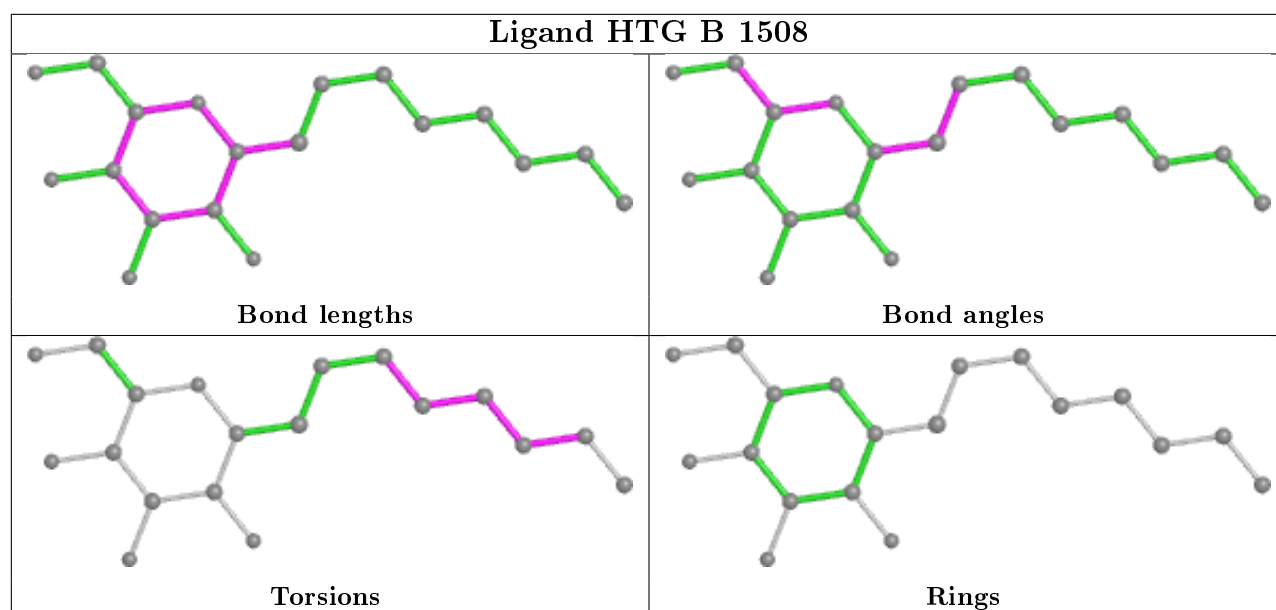
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

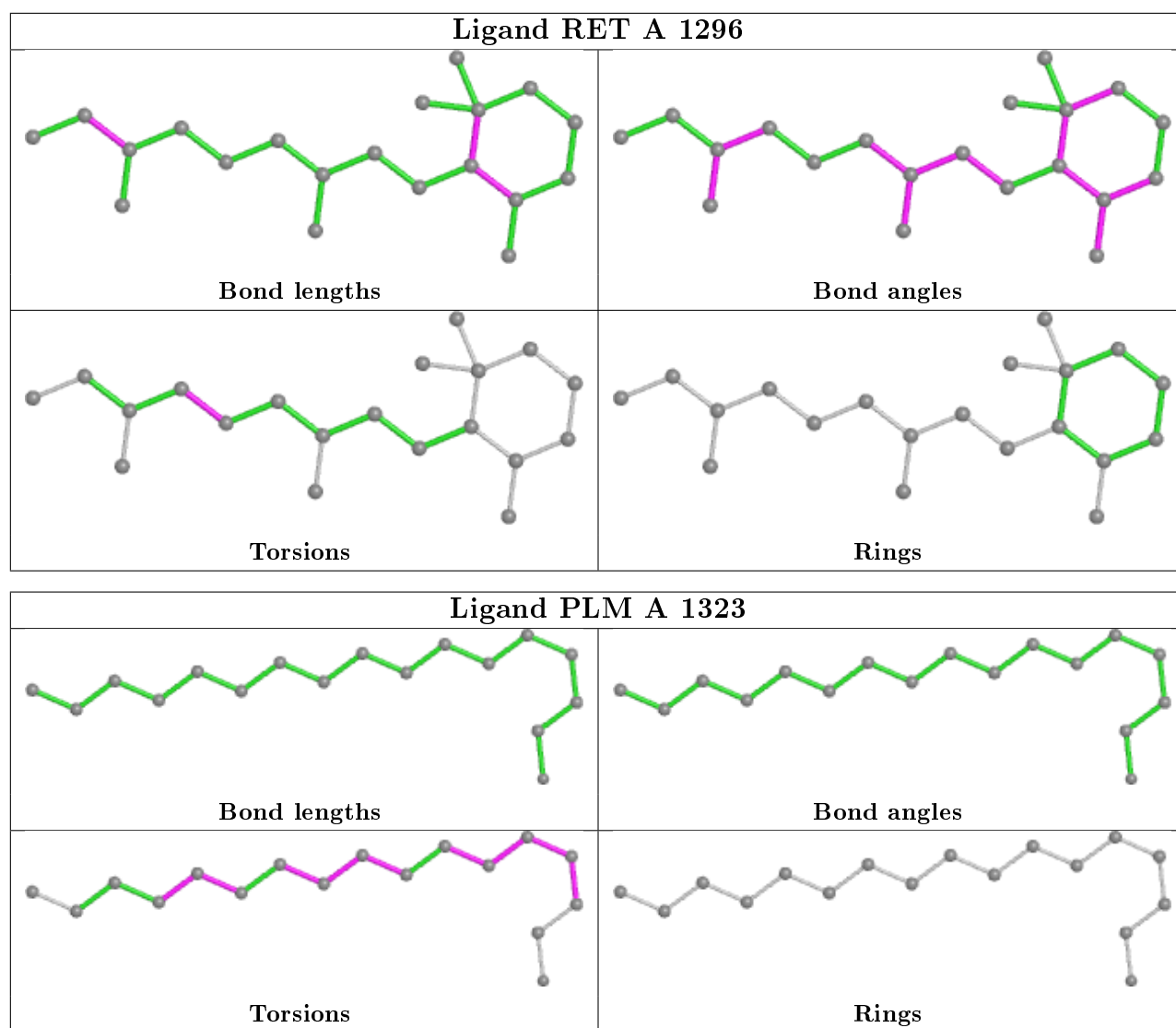












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.