



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 1FE2 / pdb\_00001fe2  
Title : CRYSTAL STRUCTURE OF DIHOMO-GAMMA-LINOLEIC ACID BOUND IN THE CYCLOOXYGENASE CHANNEL OF PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE-1.  
Authors : Thuresson, E.D.; Malkowski, M.G.; Lakkides, K.M.; Smith, W.L.; Garavito, R.M.  
Deposited on : 2000-07-20  
Resolution : 3.00 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

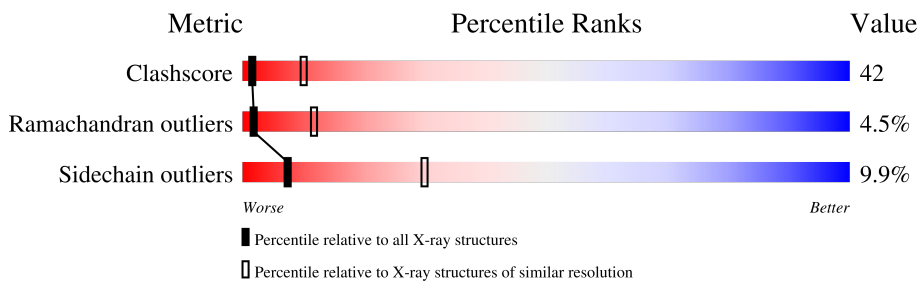
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 of 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	576	 36% 48% 11% . .
2	B	2	 100%
2	D	2	 50% 50%
3	C	5	 20% 20% 60%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2	X	-	-	-
3	BMA	C	5	X	-	-	-
4	BOG	A	751	-	-	X	-
5	COH	A	601	X	-	-	-
6	LAX	A	700	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4699 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 PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE-1.

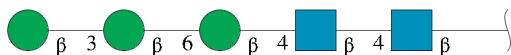
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4397	2855	734	780	28	0	0	0

- Molecule 2 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
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

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



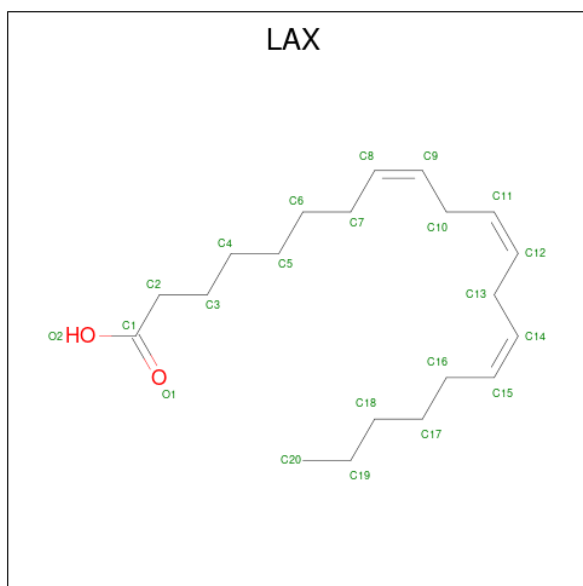
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	61	34	2	25	0	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Co	N			O
5	A	1	43	34	1	4	4	0	0

- Molecule 6 is EICOSA-8,11,14-TRIENOIC ACID (CCD ID: LAX) (formula:  $C_{20}H_{34}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	1	22	2	0	0

- Molecule 7 is water.

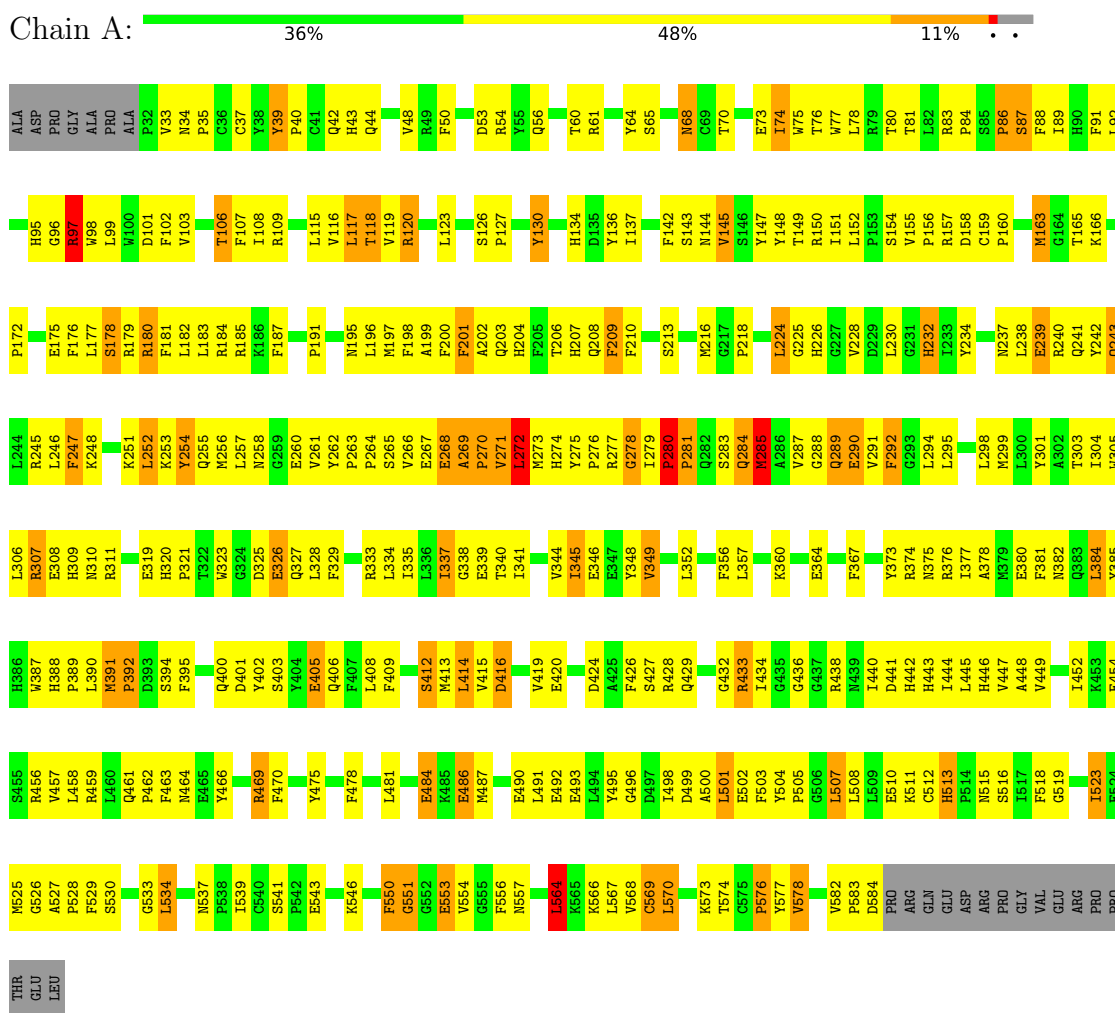
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	60	Total 60 O 60	0	0

### 3 Residue-property plots

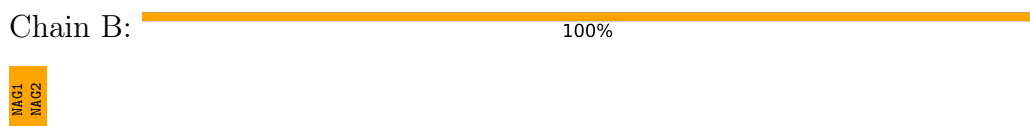
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE-1



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



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

Chain D:  50% 50%

MAG1  
MAG2

- Molecule 3: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  20% 20% 60%

MAG1  
MAG2  
BMA3  
BMA4  
BMA5

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.19Å 182.19Å 103.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.4 (20.00-3.00)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: BMA, BOG, NAG, LAX, COH

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	0.55	0/4536	1.06	30/6179 (0.5%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	LEU	N-CA-C	-8.07	102.42	111.14
1	A	143	SER	N-CA-C	7.62	122.68	113.23
1	A	148	TYR	N-CA-C	-7.50	100.63	110.53
1	A	356	PHE	N-CA-C	-7.32	103.31	112.90
1	A	232	HIS	N-CA-C	-7.15	102.37	113.02
1	A	513	HIS	N-CA-C	-6.89	101.07	109.83
1	A	391	MET	CA-C-N	6.79	128.32	119.84
1	A	391	MET	C-N-CA	6.79	128.32	119.84
1	A	285	MET	N-CA-C	6.75	120.86	110.20
1	A	345	ILE	N-CA-C	6.33	116.50	110.74
1	A	224	LEU	N-CA-C	-6.26	102.10	110.55
1	A	225	GLY	N-CA-C	-5.85	108.12	115.08
1	A	550	PHE	N-CA-C	-5.66	105.06	112.41
1	A	269	ALA	CA-C-N	5.60	126.84	119.84
1	A	269	ALA	C-N-CA	5.60	126.84	119.84
1	A	271	VAL	N-CA-C	5.56	117.93	108.86
1	A	357	LEU	N-CA-C	-5.55	102.06	110.28
1	A	337	ILE	N-CA-C	-5.54	104.16	111.09
1	A	65	SER	N-CA-C	-5.52	101.37	109.81
1	A	73	GLU	N-CA-C	-5.49	103.14	110.55
1	A	280	PRO	N-CA-C	5.41	117.30	110.70
1	A	86	PRO	N-CA-C	-5.39	106.37	113.65
1	A	175	GLU	N-CA-C	-5.33	105.39	111.14
1	A	457	VAL	N-CA-C	-5.25	105.27	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	LYS	N-CA-C	-5.16	105.82	112.68
1	A	39	TYR	CA-C-N	5.16	124.47	118.85
1	A	39	TYR	C-N-CA	5.16	124.47	118.85
1	A	412	SER	N-CA-C	-5.09	107.75	114.31
1	A	95	HIS	N-CA-C	5.07	121.59	110.80
1	A	553	GLU	N-CA-C	-5.01	105.92	112.23

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	4397	0	4203	373	0
2	B	28	0	25	3	0
2	D	28	0	25	2	0
3	C	61	0	52	3	0
4	A	60	0	84	16	0
5	A	43	0	30	2	0
6	A	22	0	33	22	0
7	A	60	0	0	7	0
All	All	4699	0	4452	383	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 42.

All (383) 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)
2:B:1:NAG:H61	2:B:2:NAG:H82	1.35	1.08
1:A:263:PRO:HD2	1:A:285:MET:HE2	1.31	1.08
1:A:97:ARG:HH21	1:A:97:ARG:HB2	1.18	1.04
1:A:98:TRP:HB2	4:A:752:BOG:H5'1	1.46	0.95
1:A:239:GLU:CD	1:A:239:GLU:H	1.75	0.94
1:A:251:LYS:HB3	1:A:310:ASN:ND2	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HB2	1:A:97:ARG:NH2	1.83	0.92
1:A:243:GLN:HG3	1:A:270:PRO:HG2	1.49	0.92
1:A:294:LEU:O	1:A:295:LEU:HG	1.70	0.90
1:A:501:LEU:HD12	1:A:502:GLU:H	1.38	0.89
1:A:163:MET:HA	1:A:163:MET:HE2	1.58	0.86
1:A:530:SER:OG	6:A:700:LAX:H132	1.76	0.85
1:A:195:ASN:ND2	1:A:427:SER:HA	1.92	0.84
1:A:391:MET:HE2	1:A:391:MET:HA	1.59	0.84
1:A:344:VAL:O	1:A:348:TYR:HB3	1.77	0.84
1:A:272:LEU:HD12	1:A:273:MET:H	1.45	0.80
1:A:87:SER:HB2	4:A:750:BOG:H62	1.63	0.79
1:A:523:ILE:HG23	6:A:700:LAX:H62	1.63	0.79
1:A:533:GLY:HA3	6:A:700:LAX:H203	1.65	0.78
1:A:89:ILE:HG23	4:A:751:BOG:H8'1	1.66	0.78
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.65	0.78
1:A:208:GLN:NE2	1:A:230:LEU:H	1.84	0.76
1:A:513:HIS:HB2	1:A:516:SER:OG	1.85	0.76
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.68	0.75
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.66	0.75
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.67	0.74
1:A:326:GLU:OE1	1:A:326:GLU:HA	1.88	0.74
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.68	0.74
1:A:273:MET:HE2	1:A:285:MET:O	1.86	0.74
1:A:526:GLY:C	6:A:700:LAX:H9	2.13	0.74
1:A:543:GLU:O	1:A:546:LYS:HE3	1.87	0.74
1:A:120:ARG:NE	4:A:751:BOG:H1	2.03	0.74
1:A:242:TYR:CD2	1:A:247:PHE:HZ	2.06	0.73
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.70	0.73
1:A:384:LEU:C	1:A:384:LEU:HD23	2.12	0.73
1:A:137:ILE:H	1:A:137:ILE:HD12	1.52	0.73
1:A:501:LEU:HD12	1:A:502:GLU:N	2.02	0.73
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.29	0.73
1:A:120:ARG:CZ	4:A:751:BOG:H1	2.18	0.72
1:A:442:HIS:CD2	1:A:443:HIS:H	2.08	0.72
1:A:89:ILE:HG23	4:A:751:BOG:C8'	2.20	0.72
1:A:391:MET:HG3	5:A:601:COH:HAB	1.72	0.71
1:A:462:PRO:HB3	1:A:499:ASP:O	1.91	0.70
1:A:272:LEU:HD12	1:A:273:MET:N	2.06	0.70
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.71	0.70
1:A:115:LEU:HD23	4:A:751:BOG:H5'2	1.72	0.70
1:A:60:THR:HG22	1:A:61:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.28	0.69
1:A:130:TYR:HB3	1:A:134:HIS:O	1.92	0.68
1:A:237:ASN:ND2	1:A:240:ARG:H	1.91	0.68
1:A:126:SER:HA	1:A:127:PRO:C	2.19	0.68
1:A:334:LEU:HD23	1:A:337:ILE:HD12	1.75	0.67
1:A:150:ARG:NH1	1:A:154:SER:HB3	2.10	0.67
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.10	0.67
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.29	0.67
1:A:172:PRO:HB2	1:A:177:LEU:HD13	1.76	0.67
1:A:512:CYS:HA	1:A:519:GLY:HA2	1.75	0.66
1:A:137:ILE:HD12	1:A:137:ILE:N	2.10	0.66
1:A:292:PHE:O	1:A:299:MET:HE2	1.95	0.66
1:A:352:LEU:HD23	6:A:700:LAX:H71	1.78	0.66
1:A:253:LYS:O	1:A:254:TYR:HB3	1.96	0.66
1:A:344:VAL:O	1:A:349:VAL:HG23	1.96	0.65
1:A:172:PRO:CB	1:A:177:LEU:HD13	2.25	0.65
1:A:412:SER:O	1:A:416:ASP:HB2	1.96	0.65
1:A:178:SER:OG	1:A:449:VAL:HG22	1.96	0.65
1:A:89:ILE:HD12	4:A:751:BOG:H8'3	1.78	0.65
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.97	0.65
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.78	0.65
6:A:700:LAX:C8	6:A:700:LAX:H41	2.27	0.65
1:A:334:LEU:HA	1:A:337:ILE:HD12	1.78	0.65
1:A:442:HIS:HD2	1:A:443:HIS:H	1.44	0.64
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.79	0.64
1:A:48:VAL:HG22	7:A:852:HOH:O	1.97	0.64
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.61	0.64
1:A:495:TYR:OH	1:A:502:GLU:HG3	1.98	0.64
1:A:102:PHE:O	1:A:106:THR:HG23	1.98	0.63
1:A:258:ASN:HD21	1:A:415:VAL:HG12	1.62	0.63
1:A:530:SER:OG	6:A:700:LAX:H101	1.98	0.63
1:A:279:ILE:HG22	1:A:279:ILE:O	1.98	0.63
1:A:414:LEU:HD12	1:A:414:LEU:O	1.99	0.63
1:A:39:TYR:OH	1:A:155:VAL:HG22	1.99	0.63
1:A:279:ILE:C	1:A:281:PRO:CD	2.72	0.63
1:A:226:HIS:HB3	1:A:377:ILE:HG12	1.81	0.63
1:A:463:PHE:HB2	1:A:502:GLU:O	1.98	0.63
1:A:202:ALA:O	1:A:206:THR:HG23	1.98	0.62
1:A:287:VAL:HG23	1:A:289:GLN:H	1.64	0.62
1:A:442:HIS:CD2	1:A:443:HIS:N	2.66	0.62
1:A:388:HIS:HB3	1:A:444:ILE:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:NAG:H61	2:B:2:NAG:C8	2.22	0.62
1:A:88:PHE:O	1:A:91:PHE:HB3	1.99	0.62
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.34	0.62
1:A:230:LEU:C	1:A:232:HIS:H	2.07	0.62
1:A:258:ASN:ND2	1:A:415:VAL:HG12	2.15	0.62
1:A:40:PRO:HB3	2:B:1:NAG:H62	1.82	0.61
1:A:207:HIS:HB3	1:A:289:GLN:HE21	1.65	0.61
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.36	0.61
1:A:237:ASN:HB2	1:A:239:GLU:OE1	2.01	0.61
1:A:444:ILE:O	1:A:447:VAL:HG23	2.00	0.61
1:A:424:ASP:O	1:A:428:ARG:HD2	2.01	0.61
1:A:255:GLN:HE21	1:A:264:PRO:HA	1.65	0.60
1:A:239:GLU:CD	1:A:239:GLU:N	2.56	0.60
1:A:265:SER:HA	1:A:285:MET:HA	1.82	0.60
1:A:564:LEU:HD22	1:A:578:VAL:CG2	2.32	0.60
1:A:352:LEU:HD23	6:A:700:LAX:C7	2.31	0.60
1:A:97:ARG:O	1:A:101:ASP:OD2	2.19	0.60
1:A:582:VAL:HG22	1:A:583:PRO:O	2.02	0.60
1:A:463:PHE:HE1	1:A:507:LEU:HG	1.66	0.60
1:A:179:ARG:HA	1:A:183:LEU:HB2	1.84	0.60
1:A:196:LEU:HD11	1:A:429:GLN:NE2	2.16	0.59
1:A:412:SER:O	1:A:416:ASP:N	2.31	0.59
1:A:109:ARG:NH2	1:A:360:LYS:HB2	2.18	0.59
1:A:120:ARG:HD2	4:A:751:BOG:O2	2.02	0.59
1:A:257:LEU:O	1:A:258:ASN:HB2	2.01	0.59
1:A:204:HIS:CD2	1:A:232:HIS:CD2	2.91	0.59
1:A:182:LEU:HB3	1:A:440:ILE:CD1	2.33	0.59
1:A:245:ARG:NH2	1:A:325:ASP:OD2	2.36	0.59
1:A:414:LEU:HD12	1:A:414:LEU:C	2.28	0.59
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.38	0.58
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.38	0.58
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.39	0.58
1:A:243:GLN:HG3	1:A:270:PRO:CG	2.29	0.58
1:A:263:PRO:HD2	1:A:285:MET:CE	2.20	0.58
1:A:237:ASN:HD21	1:A:240:ARG:HB2	1.69	0.58
1:A:86:PRO:HA	4:A:751:BOG:H62	1.84	0.58
1:A:566:LYS:O	1:A:570:LEU:HB2	2.04	0.58
1:A:96:GLY:O	1:A:98:TRP:N	2.36	0.57
1:A:185:ARG:N	1:A:185:ARG:HD2	2.18	0.57
1:A:292:PHE:CD1	1:A:298:LEU:HD23	2.40	0.57
1:A:216:MET:HG2	3:C:2:NAG:C8	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HG	1:A:246:LEU:O	2.04	0.57
1:A:337:ILE:O	1:A:341:ILE:HG13	2.04	0.57
1:A:77:TRP:O	1:A:81:THR:HG23	2.04	0.57
1:A:201:PHE:CD2	1:A:201:PHE:C	2.81	0.57
1:A:185:ARG:NH1	1:A:438:ARG:NH1	2.53	0.57
1:A:333:ARG:O	1:A:337:ILE:HG13	2.05	0.57
1:A:319:GLU:HB3	1:A:320:HIS:ND1	2.20	0.57
1:A:279:ILE:N	1:A:280:PRO:HD3	2.20	0.56
1:A:280:PRO:N	1:A:281:PRO:HD3	2.19	0.56
1:A:415:VAL:HG23	7:A:857:HOH:O	2.05	0.56
1:A:523:ILE:CG2	6:A:700:LAX:H62	2.34	0.56
1:A:201:PHE:C	1:A:201:PHE:HD2	2.12	0.56
1:A:204:HIS:CD2	1:A:232:HIS:HD2	2.23	0.56
1:A:243:GLN:CG	1:A:270:PRO:HG2	2.31	0.56
1:A:115:LEU:O	1:A:119:VAL:HG23	2.05	0.55
1:A:403:SER:N	1:A:406:GLN:OE1	2.38	0.55
1:A:484:GLU:OE2	1:A:487:MET:N	2.39	0.55
1:A:216:MET:HG2	3:C:2:NAG:H82	1.88	0.55
1:A:109:ARG:HH21	1:A:360:LYS:HB2	1.71	0.55
1:A:388:HIS:N	1:A:389:PRO:HD2	2.22	0.55
1:A:278:GLY:C	1:A:280:PRO:HD3	2.32	0.55
1:A:306:LEU:HD23	1:A:306:LEU:C	2.32	0.55
1:A:242:TYR:CD2	1:A:247:PHE:CZ	2.93	0.55
1:A:254:TYR:CD1	1:A:261:VAL:HG13	2.41	0.54
1:A:340:THR:O	1:A:344:VAL:HG23	2.08	0.54
1:A:87:SER:CB	4:A:750:BOG:H62	2.33	0.54
1:A:149:THR:O	1:A:378:ALA:HA	2.05	0.54
1:A:335:ILE:O	1:A:339:GLU:HG3	2.07	0.54
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.43	0.54
1:A:564:LEU:HD22	1:A:578:VAL:HG21	1.88	0.54
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.88	0.54
1:A:151:ILE:HG23	1:A:469:ARG:NH1	2.23	0.54
1:A:254:TYR:HD1	1:A:261:VAL:HG13	1.73	0.53
1:A:452:ILE:O	1:A:456:ARG:HG3	2.08	0.53
1:A:470:PHE:CD1	1:A:525:MET:HA	2.43	0.53
1:A:152:LEU:HD12	1:A:466:TYR:CE1	2.43	0.53
1:A:245:ARG:HB2	1:A:247:PHE:CE1	2.43	0.53
1:A:513:HIS:CE1	1:A:523:ILE:HD11	2.43	0.53
1:A:238:LEU:O	1:A:241:GLN:HB3	2.08	0.53
1:A:308:GLU:O	1:A:311:ARG:HB3	2.09	0.53
1:A:408:LEU:HB3	1:A:409:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HB3	1:A:136:TYR:CE1	2.44	0.53
1:A:320:HIS:O	1:A:323:TRP:HB2	2.08	0.53
1:A:298:LEU:N	1:A:298:LEU:HD12	2.24	0.53
1:A:40:PRO:O	1:A:68:ASN:HB3	2.08	0.53
1:A:181:PHE:O	1:A:438:ARG:N	2.42	0.53
1:A:384:LEU:C	1:A:384:LEU:CD2	2.82	0.53
1:A:226:HIS:HB3	1:A:377:ILE:H	1.74	0.52
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.44	0.52
1:A:142:PHE:O	1:A:376:ARG:NH2	2.43	0.52
1:A:195:ASN:HD22	1:A:427:SER:HA	1.73	0.52
1:A:408:LEU:HB3	1:A:409:PHE:CD1	2.44	0.52
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.45	0.52
1:A:391:MET:HA	1:A:391:MET:CE	2.37	0.52
1:A:419:VAL:O	1:A:420:GLU:C	2.52	0.52
1:A:258:ASN:ND2	1:A:415:VAL:CG1	2.73	0.52
1:A:348:TYR:CE2	6:A:700:LAX:H14	2.46	0.52
1:A:384:LEU:HD23	1:A:384:LEU:O	2.10	0.52
1:A:295:LEU:HD21	1:A:408:LEU:HD23	1.92	0.51
1:A:537:ASN:OD1	1:A:539:ILE:HG23	2.11	0.51
1:A:200:PHE:O	1:A:201:PHE:C	2.54	0.51
1:A:380:GLU:HG2	1:A:466:TYR:CZ	2.46	0.51
1:A:261:VAL:HB	1:A:307:ARG:HD2	1.93	0.51
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.41	0.51
1:A:201:PHE:HD2	1:A:201:PHE:O	1.94	0.51
1:A:530:SER:OG	6:A:700:LAX:H161	2.11	0.51
1:A:218:PRO:HB3	1:A:454:GLU:HG3	1.92	0.51
1:A:513:HIS:HB2	1:A:516:SER:CB	2.41	0.51
4:A:752:BOG:H8'2	4:A:752:BOG:C4'	2.40	0.51
1:A:89:ILE:CD1	4:A:751:BOG:H8'3	2.41	0.51
1:A:403:SER:OG	1:A:405:GLU:HG2	2.11	0.51
4:A:752:BOG:H8'2	4:A:752:BOG:H4'1	1.93	0.51
1:A:530:SER:O	1:A:534:LEU:HD22	2.11	0.50
1:A:75:TRP:CE3	1:A:78:LEU:HD12	2.46	0.50
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.75	0.50
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.47	0.50
1:A:413:MET:HA	2:D:1:NAG:O6	2.11	0.50
1:A:238:LEU:HB3	1:A:239:GLU:OE2	2.11	0.50
1:A:568:VAL:HG12	1:A:569:CYS:N	2.25	0.50
1:A:518:PHE:HZ	6:A:700:LAX:H72	1.76	0.50
1:A:228:VAL:O	1:A:337:ILE:HG23	2.12	0.49
1:A:137:ILE:H	1:A:137:ILE:CD1	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:NH1	1:A:459:ARG:HD2	2.26	0.49
1:A:201:PHE:HB2	1:A:301:TYR:CZ	2.47	0.49
1:A:309:HIS:C	1:A:309:HIS:CD2	2.89	0.49
1:A:117:LEU:O	1:A:118:THR:C	2.54	0.49
1:A:204:HIS:ND1	1:A:301:TYR:CB	2.76	0.49
1:A:120:ARG:NH1	6:A:700:LAX:O2	2.45	0.49
1:A:289:GLN:HB3	1:A:292:PHE:CD1	2.47	0.49
1:A:500:ALA:O	1:A:501:LEU:C	2.56	0.49
1:A:43:HIS:O	1:A:44:GLN:HB2	2.12	0.49
1:A:287:VAL:HG23	1:A:288:GLY:N	2.27	0.49
1:A:338:GLY:O	1:A:339:GLU:C	2.55	0.49
1:A:478:PHE:CE1	1:A:498:ILE:HA	2.48	0.49
1:A:498:ILE:HG23	1:A:499:ASP:N	2.26	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.95	0.48
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.49	0.48
1:A:373:TYR:CZ	1:A:541:SER:HA	2.48	0.48
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.95	0.48
1:A:266:VAL:HG21	1:A:284:GLN:HE22	1.78	0.48
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.39	0.48
1:A:486:GLU:O	1:A:487:MET:C	2.56	0.48
1:A:392:PRO:HG3	1:A:429:GLN:NE2	2.29	0.48
1:A:96:GLY:C	1:A:98:TRP:H	2.21	0.48
1:A:149:THR:HG22	1:A:377:ILE:O	2.13	0.48
1:A:200:PHE:O	1:A:203:GLN:N	2.47	0.48
1:A:257:LEU:O	1:A:258:ASN:CB	2.61	0.48
3:C:3:BMA:O6	3:C:4:BMA:H62	2.13	0.48
1:A:145:VAL:HG13	1:A:226:HIS:HE2	1.78	0.47
1:A:321:PRO:C	1:A:323:TRP:H	2.22	0.47
1:A:490:GLU:O	1:A:493:GLU:HB3	2.14	0.47
1:A:74:ILE:CG2	1:A:75:TRP:N	2.77	0.47
1:A:96:GLY:C	1:A:98:TRP:N	2.72	0.47
1:A:241:GLN:O	1:A:245:ARG:HG3	2.13	0.47
1:A:213:SER:OG	1:A:216:MET:HE3	2.14	0.47
1:A:458:LEU:O	1:A:459:ARG:HB2	2.13	0.47
6:A:700:LAX:H71	6:A:700:LAX:C11	2.44	0.47
1:A:305:TRP:O	1:A:308:GLU:HB3	2.15	0.47
1:A:433:ARG:NH1	1:A:436:GLY:HA3	2.29	0.47
1:A:448:ALA:O	1:A:452:ILE:HG13	2.14	0.47
1:A:478:PHE:CE2	1:A:491:LEU:HB3	2.50	0.47
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.28	0.47
1:A:413:MET:HE3	7:A:856:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:CG2	1:A:469:ARG:NH1	2.78	0.47
1:A:208:GLN:HE22	1:A:230:LEU:H	1.61	0.47
1:A:272:LEU:O	1:A:273:MET:HG2	2.13	0.47
1:A:527:ALA:N	6:A:700:LAX:H9	2.29	0.47
1:A:103:VAL:HG13	1:A:108:ILE:CG2	2.45	0.47
1:A:197:MET:HE3	1:A:301:TYR:OH	2.14	0.47
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.50	0.47
1:A:333:ARG:HG2	1:A:337:ILE:HD11	1.97	0.47
1:A:523:ILE:HA	6:A:700:LAX:H8	1.96	0.46
1:A:88:PHE:CE2	1:A:92:LEU:HD11	2.50	0.46
1:A:394:SER:C	1:A:395:PHE:CD1	2.93	0.46
1:A:267:GLU:O	1:A:268:GLU:HB2	2.14	0.46
1:A:441:ASP:OD2	1:A:442:HIS:HD2	1.97	0.46
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.50	0.46
1:A:107:PHE:C	1:A:109:ARG:N	2.71	0.46
1:A:163:MET:HA	1:A:163:MET:CE	2.40	0.46
1:A:290:GLU:CD	1:A:290:GLU:H	2.21	0.46
1:A:42:GLN:NE2	7:A:827:HOH:O	2.49	0.46
1:A:204:HIS:ND1	1:A:301:TYR:HB2	2.30	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.50	0.46
1:A:461:GLN:HB3	1:A:462:PRO:CD	2.45	0.46
1:A:74:ILE:HG22	1:A:75:TRP:N	2.30	0.45
1:A:239:GLU:N	1:A:239:GLU:OE2	2.48	0.45
1:A:279:ILE:C	1:A:281:PRO:HD3	2.41	0.45
1:A:345:ILE:HG22	1:A:346:GLU:N	2.30	0.45
1:A:183:LEU:HB2	1:A:445:LEU:HD22	1.97	0.45
1:A:490:GLU:HG3	7:A:835:HOH:O	2.15	0.45
1:A:35:PRO:C	1:A:37:CYS:H	2.25	0.45
1:A:237:ASN:OD1	1:A:240:ARG:HB3	2.17	0.45
1:A:245:ARG:HD2	1:A:329:PHE:CE2	2.52	0.45
1:A:253:LYS:O	1:A:254:TYR:CB	2.63	0.45
1:A:274:HIS:CD2	1:A:290:GLU:HB2	2.52	0.45
1:A:145:VAL:HG11	1:A:224:LEU:HB3	1.98	0.45
1:A:181:PHE:HZ	1:A:490:GLU:HG2	1.82	0.45
1:A:246:LEU:HD12	1:A:253:LYS:HG2	1.98	0.45
1:A:269:ALA:O	1:A:271:VAL:N	2.49	0.44
1:A:280:PRO:N	1:A:281:PRO:CD	2.80	0.44
1:A:107:PHE:CD2	1:A:107:PHE:N	2.85	0.44
1:A:208:GLN:HG2	1:A:209:PHE:CD1	2.52	0.44
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.53	0.44
1:A:34:ASN:HB2	1:A:158:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.53	0.44
1:A:116:VAL:O	1:A:120:ARG:HB2	2.17	0.44
1:A:200:PHE:HE2	1:A:426:PHE:CE1	2.35	0.44
1:A:523:ILE:HG22	6:A:700:LAX:C3	2.47	0.44
1:A:213:SER:CB	1:A:216:MET:HE3	2.48	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.53	0.44
1:A:191:PRO:HG2	1:A:515:ASN:O	2.17	0.44
1:A:230:LEU:C	1:A:232:HIS:N	2.75	0.44
1:A:381:PHE:HB2	1:A:529:PHE:CG	2.52	0.44
1:A:134:HIS:HB3	1:A:136:TYR:CD1	2.52	0.44
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.52	0.44
1:A:512:CYS:HA	1:A:519:GLY:CA	2.45	0.44
1:A:84:PRO:HB2	1:A:88:PHE:HD1	1.83	0.44
1:A:144:ASN:HB3	1:A:147:TYR:HD2	1.82	0.44
1:A:252:LEU:HD11	1:A:329:PHE:HE1	1.83	0.44
1:A:426:PHE:C	1:A:428:ARG:H	2.26	0.44
1:A:123:LEU:O	1:A:469:ARG:NH2	2.50	0.43
1:A:433:ARG:HG2	1:A:433:ARG:HH11	1.82	0.43
1:A:349:VAL:CG1	6:A:700:LAX:H51	2.48	0.43
1:A:103:VAL:HG13	1:A:108:ILE:HG22	2.00	0.43
1:A:276:PRO:HA	7:A:842:HOH:O	2.18	0.43
1:A:287:VAL:HG11	1:A:299:MET:HE1	1.99	0.43
1:A:201:PHE:CD2	1:A:201:PHE:O	2.71	0.43
1:A:256:MET:SD	1:A:261:VAL:HG22	2.59	0.43
1:A:327:GLN:O	1:A:328:LEU:C	2.61	0.43
1:A:106:THR:OG1	1:A:108:ILE:HG13	2.18	0.43
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.59	0.43
1:A:550:PHE:O	1:A:551:GLY:O	2.36	0.43
1:A:176:PHE:O	1:A:180:ARG:HB2	2.19	0.43
1:A:204:HIS:ND1	1:A:301:TYR:HB3	2.34	0.43
1:A:87:SER:HB2	4:A:750:BOG:C6	2.42	0.43
1:A:185:ARG:HD3	1:A:438:ARG:HD3	2.01	0.43
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.54	0.43
1:A:64:TYR:CZ	1:A:76:THR:HG21	2.54	0.42
1:A:256:MET:HE1	1:A:261:VAL:HG22	2.00	0.42
1:A:550:PHE:O	1:A:551:GLY:C	2.62	0.42
1:A:237:ASN:HD21	1:A:240:ARG:H	1.65	0.42
1:A:246:LEU:O	1:A:248:LYS:N	2.52	0.42
1:A:294:LEU:HD22	1:A:409:PHE:HD2	1.76	0.42
1:A:553:GLU:O	1:A:557:ASN:ND2	2.52	0.42
6:A:700:LAX:C8	6:A:700:LAX:C4	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HB3	1:A:232:HIS:CG	2.54	0.42
1:A:230:LEU:HA	1:A:232:HIS:ND1	2.34	0.42
1:A:523:ILE:H	1:A:523:ILE:HG13	1.56	0.42
1:A:461:GLN:HB3	1:A:462:PRO:HD2	2.02	0.42
1:A:145:VAL:HG13	1:A:226:HIS:NE2	2.34	0.42
1:A:179:ARG:O	1:A:183:LEU:HB3	2.20	0.42
1:A:502:GLU:HB2	1:A:505:PRO:HD2	2.01	0.42
1:A:568:VAL:O	1:A:570:LEU:N	2.53	0.42
1:A:75:TRP:O	1:A:78:LEU:N	2.52	0.42
1:A:352:LEU:CD2	6:A:700:LAX:H11	2.50	0.42
1:A:510:GLU:HG2	1:A:511:LYS:O	2.20	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.77	0.42
1:A:271:VAL:HG22	1:A:272:LEU:N	2.35	0.42
1:A:390:LEU:HD21	1:A:434:ILE:HD11	2.02	0.41
1:A:527:ALA:HB2	6:A:700:LAX:C4	2.50	0.41
1:A:86:PRO:HA	4:A:751:BOG:C6	2.50	0.41
1:A:178:SER:HB3	1:A:445:LEU:HD11	2.02	0.41
1:A:266:VAL:CG2	1:A:284:GLN:NE2	2.83	0.41
1:A:446:HIS:O	1:A:447:VAL:C	2.62	0.41
1:A:464:ASN:OD1	1:A:475:TYR:N	2.52	0.41
1:A:492:GLU:O	1:A:496:GLY:N	2.44	0.41
1:A:432:GLY:O	1:A:433:ARG:C	2.64	0.41
1:A:107:PHE:H	1:A:107:PHE:HD2	1.65	0.41
1:A:184:ARG:NH1	1:A:187:PHE:HD2	2.19	0.41
1:A:295:LEU:HD11	5:A:601:COH:HBB1	2.03	0.41
1:A:304:ILE:CG2	1:A:567:LEU:HG	2.51	0.41
1:A:53:ASP:OD2	1:A:54:ARG:HG3	2.20	0.41
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.97	0.41
1:A:179:ARG:HA	1:A:183:LEU:CB	2.49	0.41
1:A:199:ALA:HB1	1:A:391:MET:HE3	2.02	0.41
1:A:266:VAL:CG2	1:A:284:GLN:HE22	2.33	0.41
1:A:375:ASN:HD22	1:A:375:ASN:HA	1.71	0.41
1:A:35:PRO:C	1:A:37:CYS:N	2.78	0.41
1:A:251:LYS:HD3	1:A:310:ASN:HD22	1.85	0.41
1:A:500:ALA:O	1:A:501:LEU:O	2.39	0.41
1:A:275:TYR:CG	1:A:284:GLN:HG2	2.55	0.40
1:A:299:MET:HG3	1:A:414:LEU:HD23	2.03	0.40
1:A:442:HIS:NE2	1:A:443:HIS:CE1	2.89	0.40
1:A:196:LEU:HD21	1:A:392:PRO:HD3	2.03	0.40
1:A:289:GLN:HB3	1:A:292:PHE:CG	2.56	0.40
1:A:255:GLN:NE2	1:A:265:SER:N	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.48	0.40
1:A:279:ILE:N	1:A:280:PRO:CD	2.85	0.40
1:A:303:THR:O	1:A:307:ARG:HB2	2.22	0.40
7:A:850:HOH:O	2:D:2:NAG:H2	2.21	0.40
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.03	0.40
6:A:700:LAX:H132	6:A:700:LAX:H101	1.79	0.40
1:A:50:PHE:CE2	1:A:56:GLN:NE2	2.89	0.40
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.53	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 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	551/576 (96%)	430 (78%)	96 (17%)	25 (4%)	<b>2</b> <b>12</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	247	PHE
1	A	281	PRO
1	A	97	ARG
1	A	178	SER
1	A	268	GLU
1	A	277	ARG
1	A	292	PHE
1	A	501	LEU
1	A	551	GLY
1	A	569	CYS
1	A	272	LEU
1	A	278	GLY

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Mol	Chain	Res	Type
1	A	486	GLU
1	A	254	TYR
1	A	118	THR
1	A	160	PRO
1	A	400	GLN
1	A	401	ASP
1	A	576	PRO
1	A	280	PRO
1	A	392	PRO
1	A	481	LEU
1	A	145	VAL
1	A	270	PRO

### 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 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	466/506 (92%)	420 (90%)	46 (10%)	<b>7</b> <b>30</b>

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	68	ASN
1	A	70	THR
1	A	74	ILE
1	A	80	THR
1	A	87	SER
1	A	97	ARG
1	A	99	LEU
1	A	106	THR
1	A	120	ARG
1	A	130	TYR
1	A	163	MET
1	A	180	ARG
1	A	201	PHE

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Mol	Chain	Res	Type
1	A	209	PHE
1	A	239	GLU
1	A	243	GLN
1	A	252	LEU
1	A	272	LEU
1	A	283	SER
1	A	284	GLN
1	A	285	MET
1	A	289	GLN
1	A	290	GLU
1	A	307	ARG
1	A	326	GLU
1	A	349	VAL
1	A	374	ARG
1	A	384	LEU
1	A	385	TYR
1	A	405	GLU
1	A	414	LEU
1	A	416	ASP
1	A	433	ARG
1	A	469	ARG
1	A	484	GLU
1	A	507	LEU
1	A	523	ILE
1	A	534	LEU
1	A	554	VAL
1	A	556	PHE
1	A	564	LEU
1	A	570	LEU
1	A	574	THR
1	A	578	VAL
1	A	584	ASP

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

Mol	Chain	Res	Type
1	A	42	GLN
1	A	43	HIS
1	A	56	GLN
1	A	203	GLN
1	A	208	GLN
1	A	232	HIS

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	255	GLN
1	A	258	ASN
1	A	274	HIS
1	A	284	GLN
1	A	310	ASN
1	A	327	GLN
1	A	375	ASN
1	A	443	HIS
1	A	557	ASN
1	A	571	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

9 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	B	1	1,2	14,14,15	0.67	0	17,19,21	1.21	1 (5%)
2	NAG	B	2	2	14,14,15	0.86	0	17,19,21	1.18	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.61	0	17,19,21	0.86	0
3	NAG	C	2	3	14,14,15	1.14	1 (7%)	17,19,21	1.43	3 (17%)
3	BMA	C	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.10	2 (13%)
3	BMA	C	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	C	5	3	11,11,12	0.89	0	15,15,17	0.77	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.68	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.74	0	17,19,21	1.06	1 (5%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	5/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	2/2/19/22	1/1/1/1
3	BMA	C	5	3	1/1/4/5	1/2/19/22	1/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	2.23	1.57	1.52
3	C	2	NAG	O4-C4	2.21	1.48	1.43
3	C	4	BMA	C1-C2	2.02	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C4-C3-C2	-3.46	105.95	111.02
3	C	2	NAG	C4-C3-C2	-3.42	106.01	111.02
2	D	2	NAG	C2-N2-C7	-3.23	118.57	122.90
3	C	3	BMA	C1-C2-C3	3.14	114.22	109.64
3	C	4	BMA	C1-O5-C5	3.11	116.36	112.19
2	B	2	NAG	C4-C3-C2	3.04	115.47	111.02
3	C	2	NAG	C1-C2-N2	2.86	114.94	110.43
3	C	2	NAG	O5-C1-C2	-2.47	107.47	111.29
3	C	3	BMA	C1-O5-C5	2.34	115.33	112.19
3	C	5	BMA	C1-O5-C5	2.19	115.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	BMA	O3-C3-C2	2.06	114.26	110.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1
3	C	5	BMA	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
3	C	4	BMA	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	5	BMA	O5-C5-C6-O6
3	C	4	BMA	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	B	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

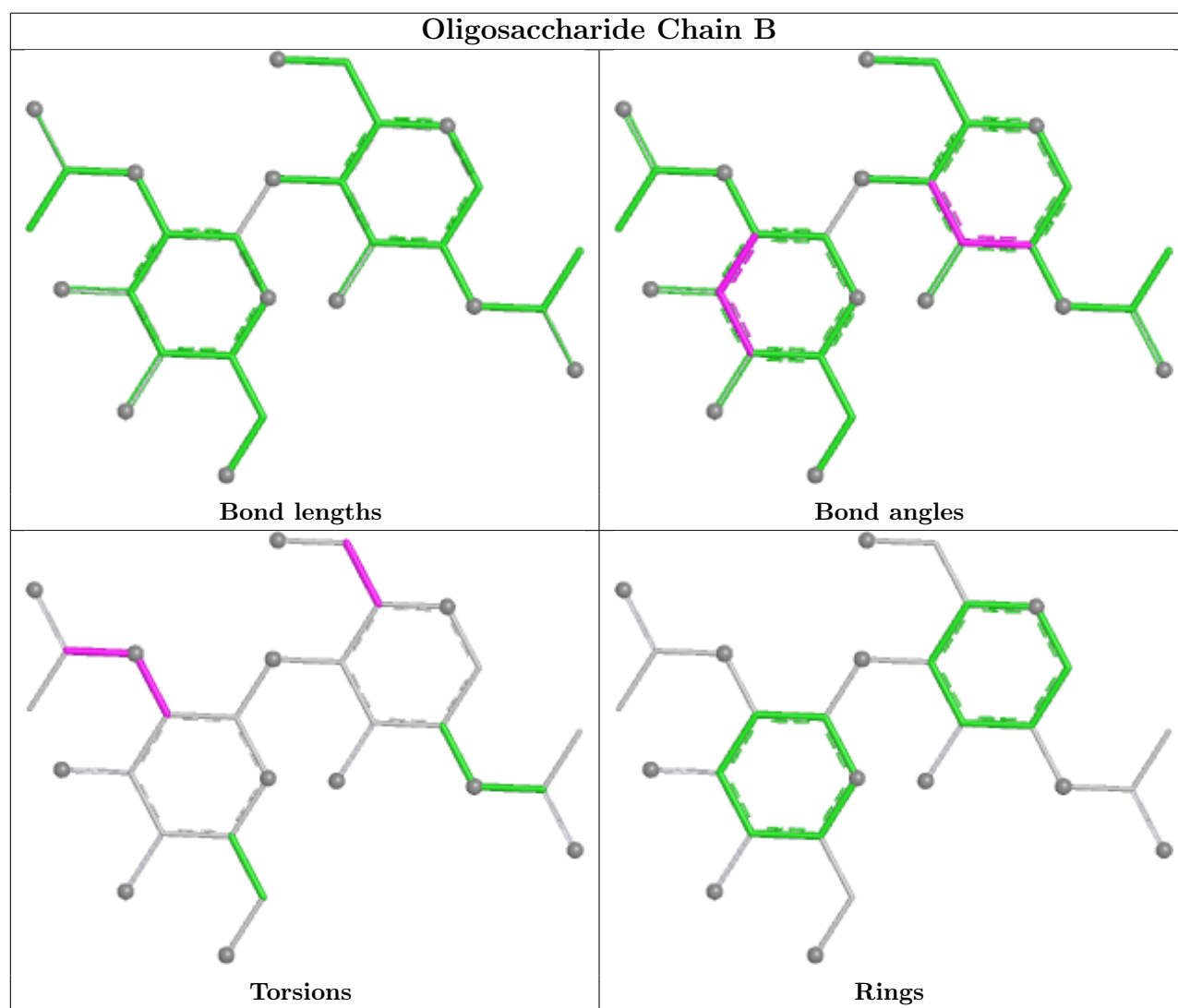
All (2) ring outliers are listed below:

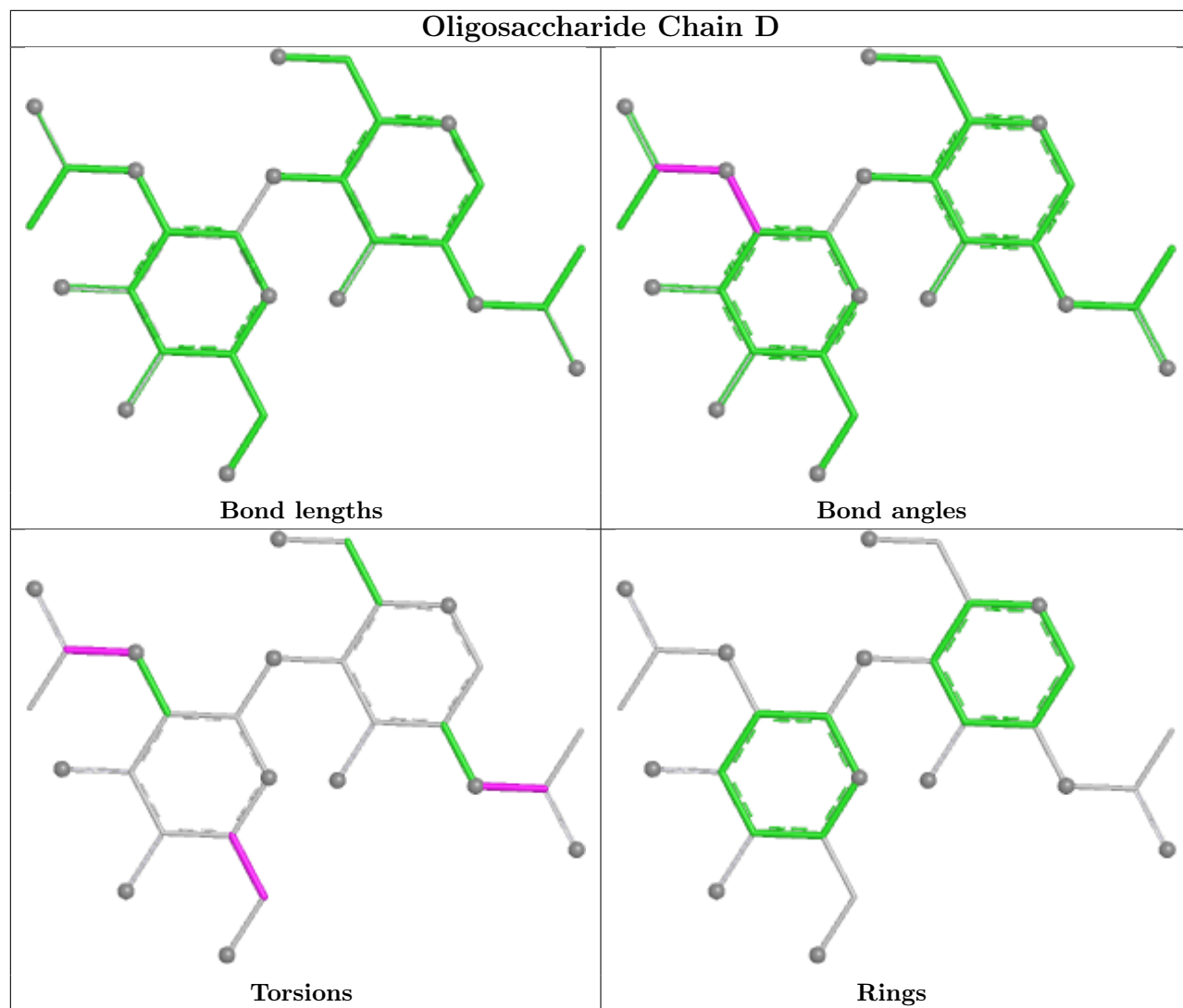
Mol	Chain	Res	Type	Atoms
3	C	5	BMA	C1-C2-C3-C4-C5-O5
3	C	4	BMA	C1-C2-C3-C4-C5-O5

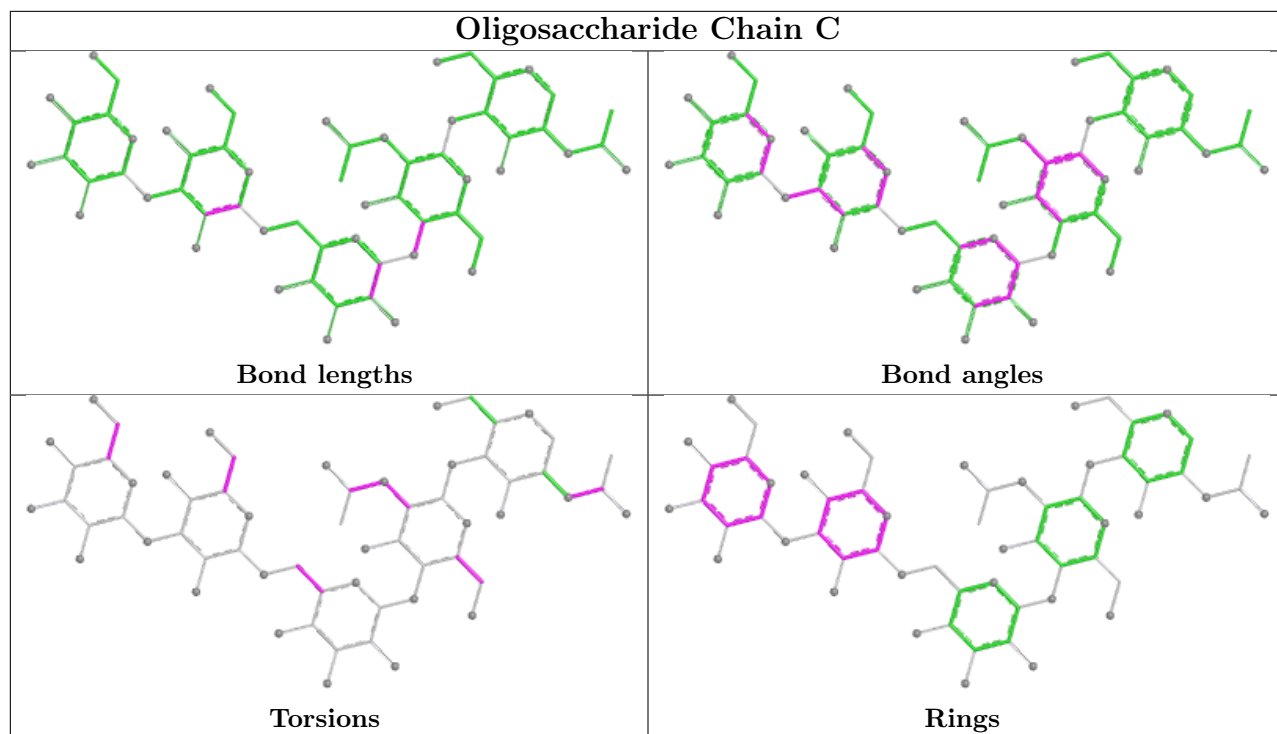
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	3	0
3	C	3	BMA	1	0
2	D	2	NAG	1	0
3	C	2	NAG	2	0
2	B	2	NAG	2	0
3	C	4	BMA	1	0
2	D	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 [i](#)

5 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	$\# Z  > 2$
5	COH	A	601	1	50,50,50	2.10	13 (26%)	66,82,82	1.65	14 (21%)
6	LAX	A	700	-	21,21,21	0.70	0	21,21,21	0.90	0
4	BOG	A	752	-	20,20,20	0.69	0	25,25,25	0.71	0
4	BOG	A	750	-	20,20,20	0.54	0	25,25,25	0.54	0
4	BOG	A	751	-	20,20,20	0.48	0	25,25,25	0.96	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	COH	A	601	1	1/1/3/9	8/14/54/54	-
6	LAX	A	700	-	-	6/19/19/19	-
4	BOG	A	752	-	-	8/11/31/31	0/1/1/1
4	BOG	A	750	-	-	6/11/31/31	0/1/1/1
4	BOG	A	751	-	-	6/11/31/31	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COH	C1D-C2D	5.55	1.56	1.43
5	A	601	COH	C1A-C2A	5.45	1.54	1.45
5	A	601	COH	C4A-C3A	5.30	1.55	1.44
5	A	601	COH	CAA-C2A	3.91	1.61	1.51
5	A	601	COH	C2A-C3A	3.73	1.44	1.36
5	A	601	COH	C4D-ND	3.61	1.44	1.38
5	A	601	COH	CMC-C2C	3.14	1.57	1.50
5	A	601	COH	CBC-CAC	2.99	1.44	1.30
5	A	601	COH	C4C-NC	-2.59	1.35	1.39
5	A	601	COH	C1A-NA	2.27	1.43	1.39
5	A	601	COH	C1D-ND	-2.19	1.35	1.38
5	A	601	COH	CHB-C4A	-2.08	1.34	1.39
5	A	601	COH	CAD-C3D	2.08	1.56	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	COH	C2B-C1B-NB	4.62	114.47	110.88
5	A	601	COH	CMD-C2D-C3D	3.91	133.91	125.62
5	A	601	COH	C4A-C3A-C2A	-3.59	103.21	106.98
5	A	601	COH	C3A-C4A-NA	3.58	114.68	110.96
4	A	751	BOG	C1'-O1-C1	3.34	119.39	113.68
5	A	601	COH	CAA-C2A-C1A	3.13	130.16	124.70
5	A	601	COH	C4B-NB-C1B	-2.80	100.98	105.11
5	A	601	COH	C4C-C3C-C2C	-2.72	104.78	107.28
5	A	601	COH	C2D-C1D-ND	2.69	112.31	109.69
5	A	601	COH	CHC-C4B-NB	-2.60	121.77	124.85
5	A	601	COH	C1D-C2D-C3D	-2.48	103.97	106.82
5	A	601	COH	CHB-C1B-NB	-2.26	122.17	124.85
5	A	601	COH	CMD-C2D-C1D	-2.17	122.11	125.42
4	A	751	BOG	O1-C1-C2	2.11	111.48	108.27
5	A	601	COH	CHB-C4A-C3A	-2.10	121.72	125.03
5	A	601	COH	C3B-C2B-C1B	-2.09	105.07	107.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	COH	NB

All (34) torsion outliers are listed below:

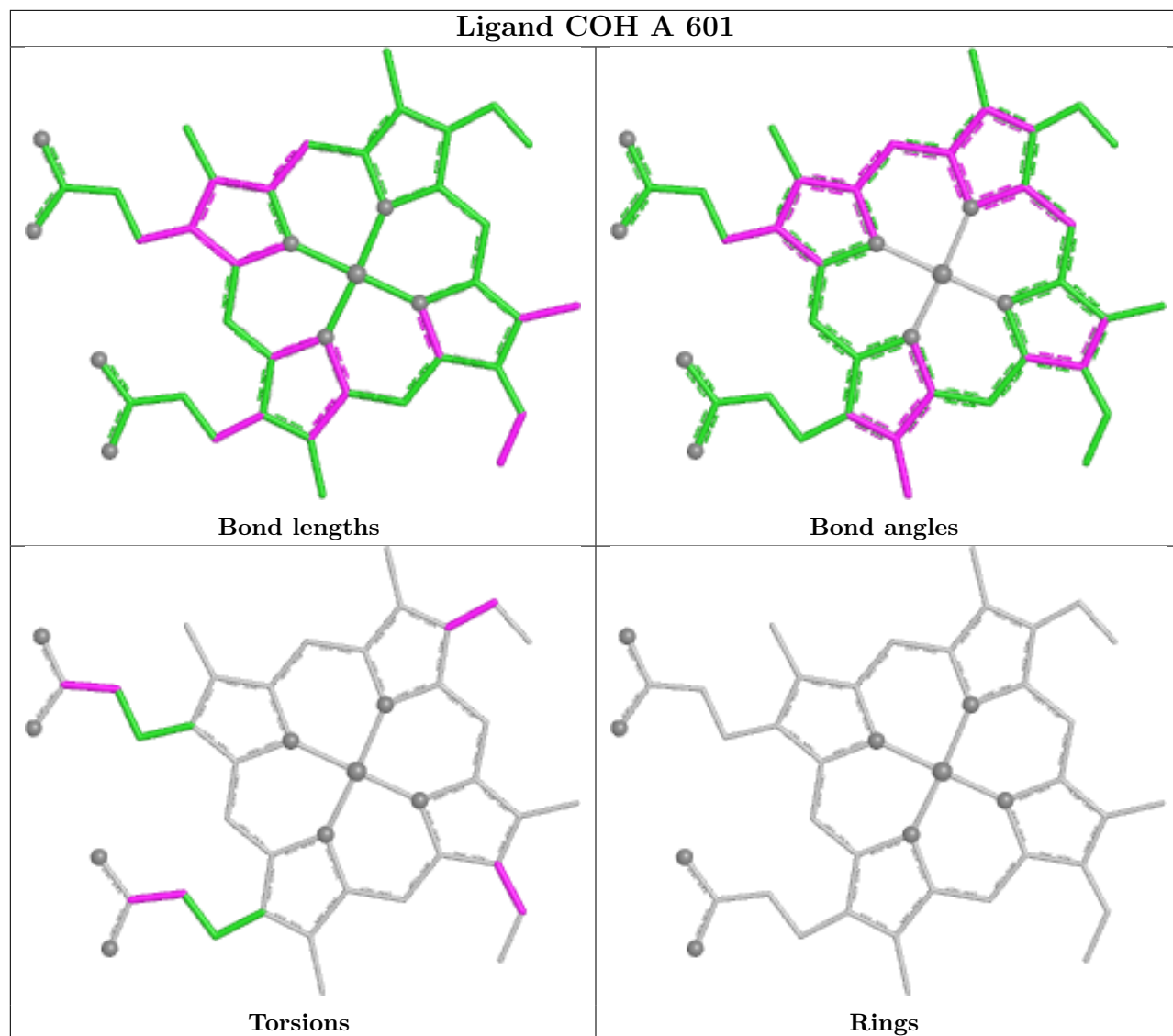
Mol	Chain	Res	Type	Atoms
4	A	751	BOG	O5-C1-O1-C1'
4	A	752	BOG	C2-C1-O1-C1'
4	A	752	BOG	O5-C1-O1-C1'
4	A	752	BOG	C2'-C1'-O1-C1
4	A	750	BOG	C4-C5-C6-O6
4	A	750	BOG	O5-C5-C6-O6
4	A	752	BOG	C4-C5-C6-O6
4	A	751	BOG	C2-C1-O1-C1'
4	A	752	BOG	O5-C5-C6-O6
4	A	751	BOG	C4-C5-C6-O6
6	A	700	LAX	C1-C2-C3-C4
6	A	700	LAX	C3-C4-C5-C6
4	A	751	BOG	O5-C5-C6-O6
4	A	750	BOG	C1'-C2'-C3'-C4'
5	A	601	COH	C2C-C3C-CAC-CBC
4	A	751	BOG	C2'-C1'-O1-C1
6	A	700	LAX	C12-C13-C14-C15
5	A	601	COH	C2B-C3B-CAB-CBB
4	A	752	BOG	C4'-C5'-C6'-C7'
5	A	601	COH	C4C-C3C-CAC-CBC
4	A	752	BOG	C5'-C6'-C7'-C8'
4	A	750	BOG	C2'-C3'-C4'-C5'
5	A	601	COH	C4B-C3B-CAB-CBB
4	A	752	BOG	C1'-C2'-C3'-C4'
6	A	700	LAX	O1-C1-C2-C3
6	A	700	LAX	O2-C1-C2-C3
5	A	601	COH	CAA-CBA-CGA-O2A
4	A	751	BOG	C4'-C5'-C6'-C7'
5	A	601	COH	CAD-CBD-CGD-O2D
6	A	700	LAX	C2-C3-C4-C5
5	A	601	COH	CAA-CBA-CGA-O1A
5	A	601	COH	CAD-CBD-CGD-O1D
4	A	750	BOG	O5-C1-O1-C1'
4	A	750	BOG	C2-C1-O1-C1'

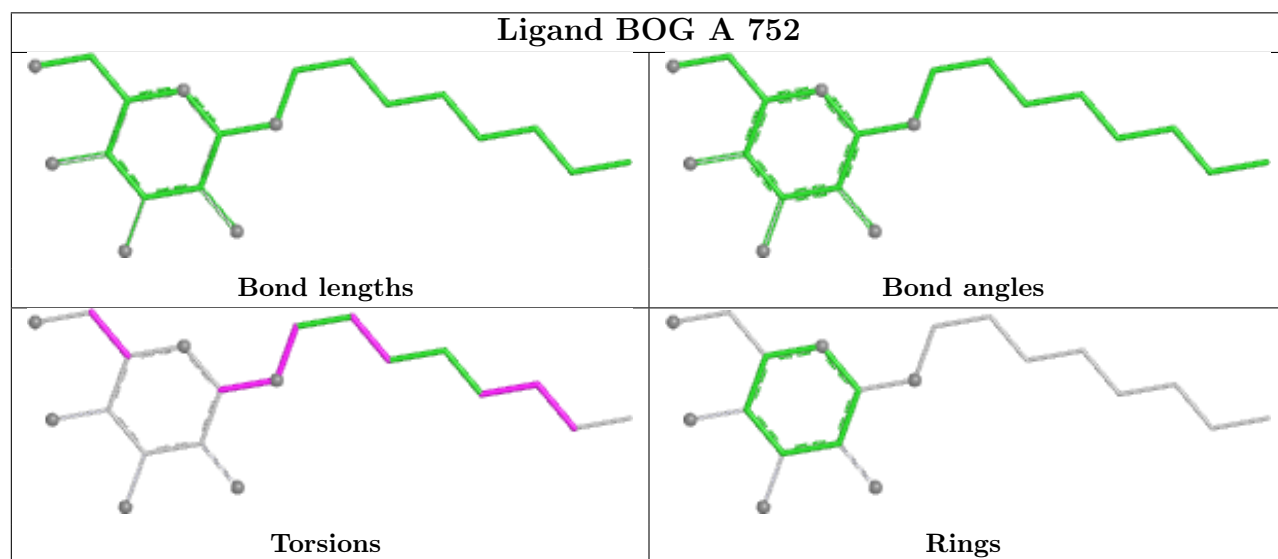
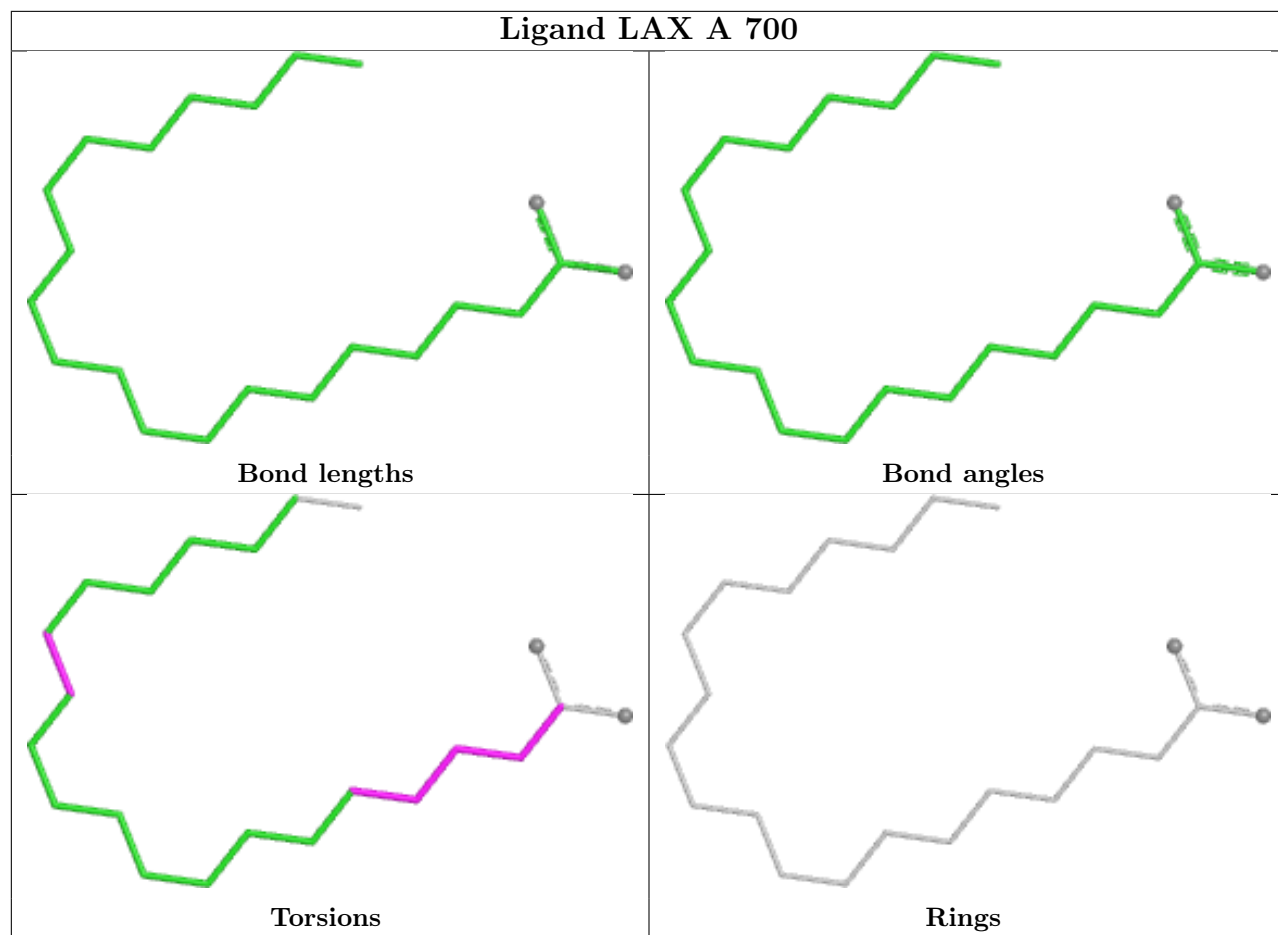
There are no ring outliers.

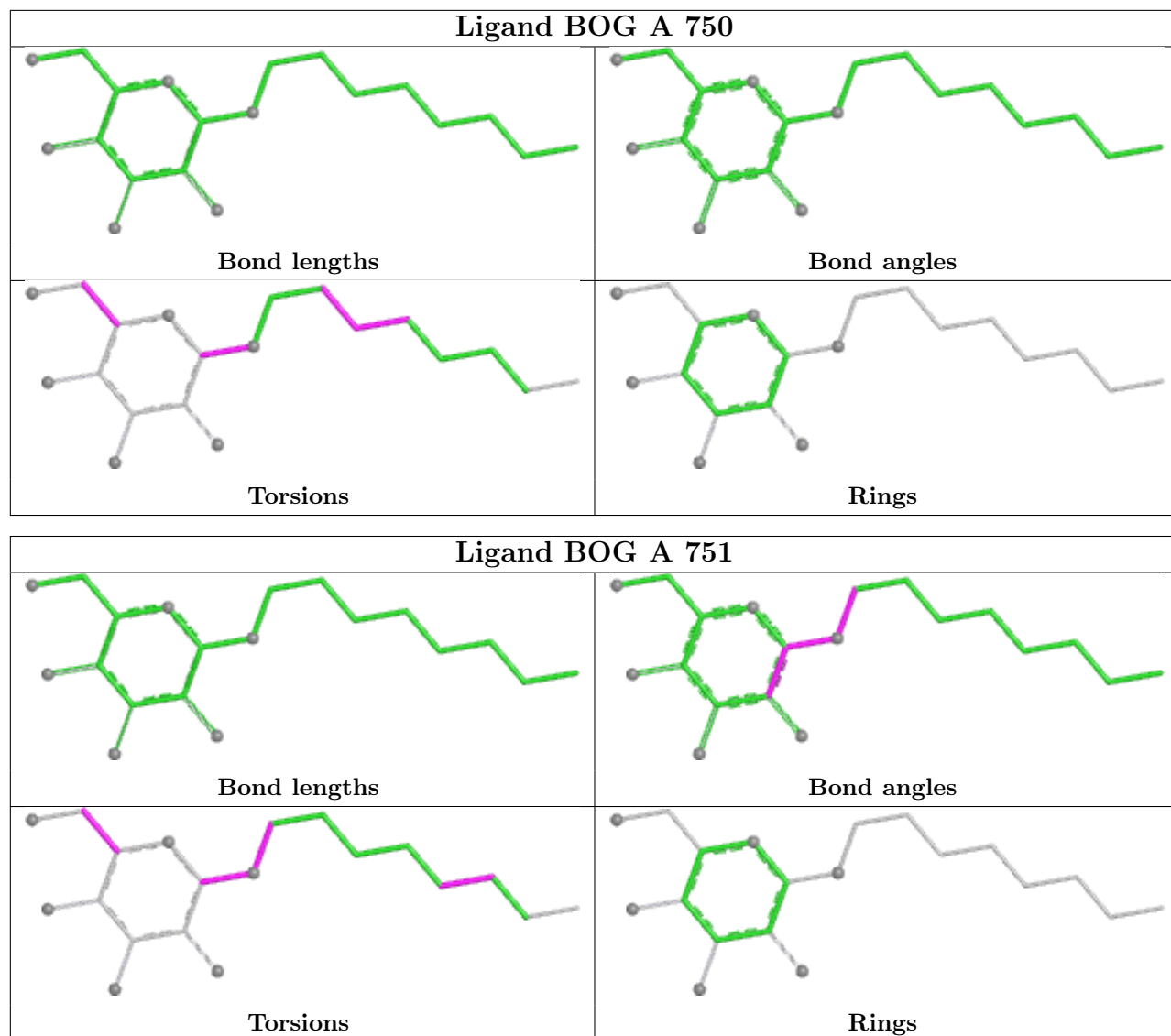
5 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	COH	2	0
6	A	700	LAX	22	0
4	A	752	BOG	3	0
4	A	750	BOG	3	0
4	A	751	BOG	10	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.