



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:26 AM BST

PDB ID : 1DIY  
Title : CRYSTAL STRUCTURE OF ARACHIDONIC ACID BOUND IN THE CYCLOOXYGENASE ACTIVE SITE OF PGHS-1  
Authors : Malkowski, M.G.; Ginell, S.L.; Smith, W.L.; Garavito, R.M.  
Deposited on : 1999-11-30  
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.

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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) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

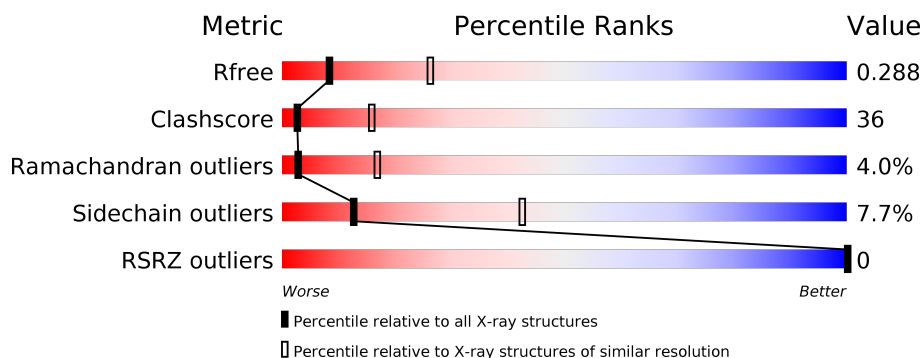
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	<div> <div style="width: 45%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> </div>
2	B	2	<div> <div style="width: 100%; background-color: orange;"></div> </div>
3	C	5	<div> <div style="width: 80%; background-color: yellow;"></div> <div style="width: 20%; background-color: orange;"></div> </div>
4	D	2	<div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 50%; background-color: orange;"></div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ACD	A	700	-	-	X	-

## 2 Entry composition [i](#)

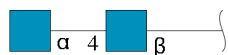
There are 8 unique types of molecules in this entry. The entry contains 4780 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 H2 SYNTHASE-1.

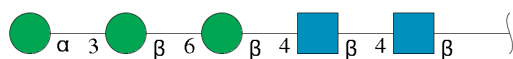
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4409	2864	741	776	28			

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



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

- Molecule 3 is an oligosaccharide called alpha-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.



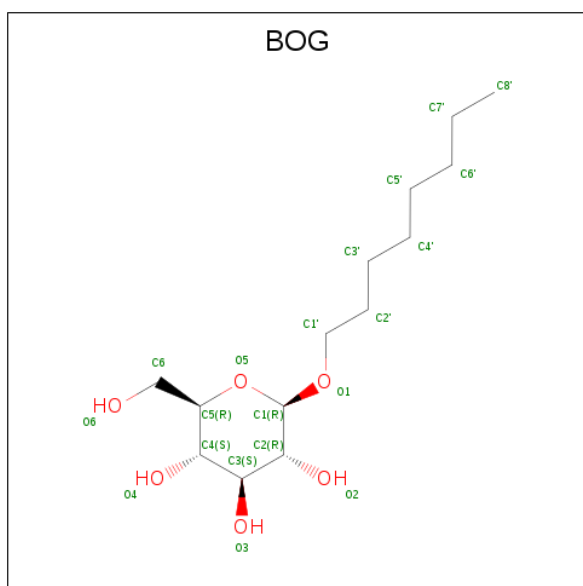
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



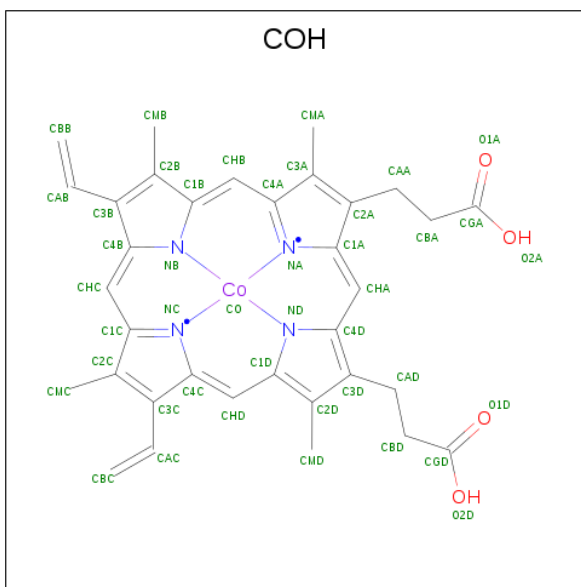
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



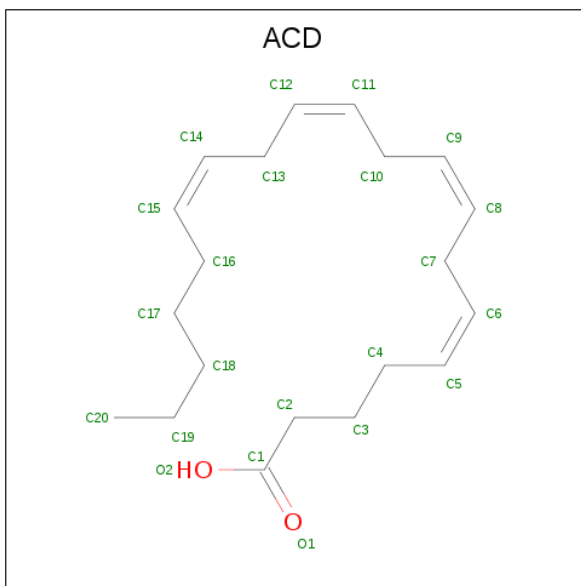
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula:  $C_{34}H_{32}CoN_4O_4$ ).



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

- Molecule 7 is ARACHIDONIC ACID (three-letter code: ACD) (formula:  $C_{20}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C O	0	0
			22	20 2		

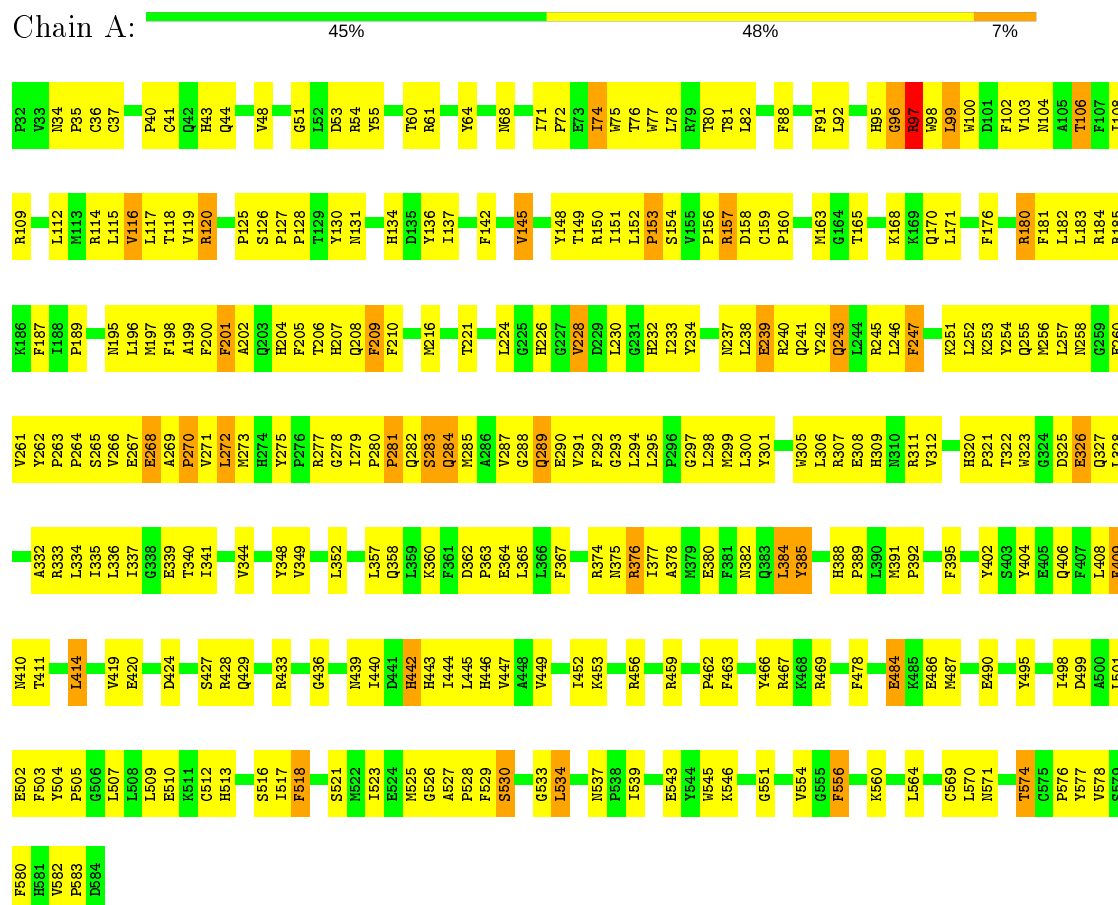
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total 109	O 109	0	0

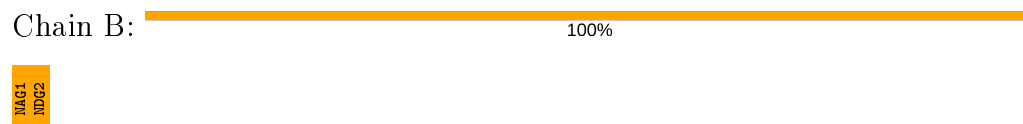
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1




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



#### • Molecule 3: alpha-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



ose

Chain C:  80% 20%

MAG1  
MAG2  
BMA3  
BMA4  
MAN5

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

Chain D:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.10Å 182.10Å 103.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 3.00 9.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (9.00-3.00) 96.6 (9.01-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.29 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.290 0.217 , 0.288	Depositor DCC
$R_{free}$ test set	959 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ACD, NDG, COH, BOG, 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	0.43	0/4548	0.68	0/6189

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4409	0	4243	327	0
2	B	28	0	24	3	0
3	C	61	0	52	1	0
4	D	28	0	25	1	0
5	A	80	0	112	11	0
6	A	43	0	30	1	0
7	A	22	0	31	13	0
8	A	109	0	0	18	0
All	All	4780	0	4517	331	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 36.

All (331) 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:97:ARG:HH21	1:A:97:ARG:HB2	1.22	1.04
1:A:469:ARG:HD3	8:A:869:HOH:O	1.57	1.02
1:A:374:ARG:HD3	8:A:877:HOH:O	1.62	0.99
1:A:501:LEU:HD12	1:A:502:GLU:H	1.24	0.99
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.51	0.92
1:A:97:ARG:NH2	1:A:97:ARG:HB2	1.83	0.92
1:A:239:GLU:CD	1:A:239:GLU:H	1.74	0.89
1:A:348:TYR:HE2	7:A:700:ACD:H12	1.40	0.85
1:A:442:HIS:CD2	1:A:443:HIS:H	1.96	0.83
1:A:202:ALA:O	1:A:206:THR:HG23	1.78	0.83
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.62	0.81
1:A:530:SER:OG	7:A:700:ACD:H132	1.80	0.81
1:A:243:GLN:HG3	1:A:270:PRO:HG2	1.62	0.81
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.65	0.79
1:A:92:LEU:HD23	5:A:753:BOG:H4'2	1.64	0.79
1:A:92:LEU:HG	5:A:753:BOG:H2'2	1.64	0.79
1:A:501:LEU:HD12	1:A:502:GLU:N	1.96	0.79
1:A:77:TRP:O	1:A:81:THR:HG23	1.83	0.78
1:A:208:GLN:NE2	1:A:230:LEU:H	1.82	0.77
1:A:119:VAL:HG12	5:A:751:BOG:C6	2.16	0.76
1:A:344:VAL:O	1:A:348:TYR:HB3	1.86	0.76
1:A:103:VAL:HG13	1:A:108:ILE:HG22	1.70	0.74
1:A:163:MET:HE2	1:A:163:MET:HA	1.70	0.73
1:A:459:ARG:HD3	8:A:846:HOH:O	1.87	0.73
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.70	0.73
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.25	0.71
1:A:543:GLU:O	1:A:546:LYS:HE3	1.91	0.71
1:A:142:PHE:O	1:A:376:ARG:NH2	2.23	0.71
1:A:40:PRO:HB3	2:B:1:NAG:H62	1.72	0.71
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.72	0.71
1:A:237:ASN:ND2	1:A:240:ARG:H	1.89	0.70
1:A:323:TRP:HE3	1:A:328:LEU:HD23	1.55	0.70
1:A:484:GLU:OE2	1:A:487:MET:N	2.24	0.70
1:A:326:GLU:OE1	1:A:326:GLU:HA	1.92	0.69
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.27	0.69
1:A:279:ILE:HG22	1:A:281:PRO:HD2	1.74	0.68
1:A:253:LYS:O	1:A:264:PRO:HD3	1.94	0.68
1:A:256:MET:O	1:A:257:LEU:HD23	1.94	0.67
1:A:48:VAL:HG13	8:A:832:HOH:O	1.93	0.67
1:A:242:TYR:CD2	1:A:247:PHE:HZ	2.12	0.67
1:A:533:GLY:HA3	7:A:700:ACD:H203	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:HIS:CD2	1:A:443:HIS:N	2.62	0.66
1:A:88:PHE:O	1:A:91:PHE:HB3	1.95	0.66
1:A:130:TYR:HB3	1:A:134:HIS:O	1.96	0.66
1:A:208:GLN:HE22	1:A:230:LEU:H	1.42	0.66
1:A:150:ARG:HD3	1:A:152:LEU:O	1.95	0.66
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.31	0.66
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.79	0.65
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.32	0.65
1:A:163:MET:HA	1:A:163:MET:CE	2.27	0.65
1:A:96:GLY:O	1:A:98:TRP:N	2.30	0.65
1:A:152:LEU:HD12	1:A:466:TYR:CZ	2.32	0.65
1:A:280:PRO:N	1:A:281:PRO:HD3	2.12	0.64
1:A:152:LEU:HD12	1:A:466:TYR:CE1	2.31	0.64
1:A:384:LEU:HD23	1:A:384:LEU:C	2.18	0.64
1:A:279:ILE:CG2	1:A:281:PRO:HD2	2.28	0.63
1:A:556:PHE:CD1	1:A:560:LYS:HE3	2.33	0.63
1:A:513:HIS:HB2	1:A:516:SER:OG	1.97	0.63
1:A:279:ILE:C	1:A:281:PRO:CD	2.67	0.63
1:A:255:GLN:OE1	1:A:257:LEU:HD21	1.99	0.62
1:A:103:VAL:HG13	1:A:108:ILE:CG2	2.29	0.62
1:A:388:HIS:N	1:A:389:PRO:HD2	2.15	0.62
1:A:145:VAL:HG13	1:A:226:HIS:NE2	2.15	0.62
1:A:183:LEU:HD13	1:A:445:LEU:HD22	1.81	0.62
1:A:237:ASN:HB2	1:A:239:GLU:OE1	1.99	0.62
1:A:459:ARG:HG2	1:A:459:ARG:HH21	1.63	0.62
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.34	0.62
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.64	0.61
1:A:53:ASP:OD2	1:A:54:ARG:HG3	2.00	0.61
1:A:537:ASN:OD1	1:A:539:ILE:HG23	2.00	0.61
1:A:126:SER:HA	1:A:127:PRO:C	2.20	0.61
1:A:433:ARG:HD2	1:A:512:CYS:SG	2.41	0.61
1:A:128:PRO:HD2	8:A:877:HOH:O	2.00	0.61
1:A:243:GLN:CG	1:A:270:PRO:HG2	2.31	0.61
1:A:287:VAL:HG23	1:A:289:GLN:H	1.65	0.61
1:A:442:HIS:NE2	1:A:443:HIS:CE1	2.68	0.61
1:A:127:PRO:HA	8:A:877:HOH:O	2.00	0.61
1:A:171:LEU:HB3	1:A:456:ARG:NH2	2.15	0.61
1:A:119:VAL:HG12	5:A:751:BOG:H61	1.83	0.60
1:A:291:VAL:O	1:A:291:VAL:HG22	2.00	0.60
1:A:582:VAL:HG22	1:A:583:PRO:O	2.00	0.60
1:A:207:HIS:HB3	1:A:289:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLN:HG3	8:A:878:HOH:O	2.01	0.60
1:A:334:LEU:HD23	1:A:337:ILE:HD12	1.84	0.60
1:A:272:LEU:HD12	1:A:273:MET:N	2.16	0.60
1:A:257:LEU:O	1:A:258:ASN:HB2	2.00	0.60
1:A:149:THR:O	1:A:378:ALA:HA	2.02	0.60
1:A:151:ILE:HD11	1:A:529:PHE:HE2	1.65	0.59
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.84	0.59
1:A:109:ARG:HH21	1:A:360:LYS:HB2	1.67	0.59
1:A:409:PHE:O	1:A:411:THR:HG23	2.03	0.59
1:A:266:VAL:HA	1:A:269:ALA:O	2.02	0.59
1:A:195:ASN:ND2	1:A:427:SER:HA	2.17	0.59
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.37	0.59
1:A:176:PHE:CZ	1:A:180:ARG:HG3	2.38	0.58
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.33	0.58
1:A:349:VAL:HG13	7:A:700:ACD:H42	1.85	0.58
1:A:171:LEU:HD13	1:A:456:ARG:HE	1.69	0.58
1:A:299:MET:HG3	1:A:414:LEU:HD23	1.85	0.58
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.32	0.58
1:A:424:ASP:O	1:A:428:ARG:HD2	2.03	0.58
1:A:204:HIS:CD2	1:A:232:HIS:CD2	2.91	0.58
1:A:60:THR:HG22	1:A:61:ARG:HG3	1.86	0.58
1:A:43:HIS:O	1:A:44:GLN:HB2	2.04	0.57
1:A:237:ASN:HD21	1:A:240:ARG:H	1.51	0.57
1:A:433:ARG:NH1	1:A:436:GLY:HA3	2.19	0.57
1:A:228:VAL:HG23	8:A:812:HOH:O	2.05	0.57
1:A:289:GLN:HB3	1:A:292:PHE:CD1	2.38	0.57
1:A:307:ARG:HD2	8:A:895:HOH:O	2.04	0.57
1:A:380:GLU:HG2	1:A:466:TYR:CZ	2.40	0.57
1:A:452:ILE:O	1:A:456:ARG:HG3	2.04	0.57
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.40	0.57
1:A:120:ARG:NH1	7:A:700:ACD:O1	2.36	0.56
1:A:102:PHE:O	1:A:106:THR:HG23	2.04	0.56
1:A:442:HIS:HD2	1:A:443:HIS:H	1.51	0.56
1:A:295:LEU:CD2	1:A:408:LEU:HD23	2.36	0.56
1:A:408:LEU:HB3	1:A:409:PHE:CD1	2.39	0.56
1:A:145:VAL:HG12	1:A:224:LEU:CD2	2.36	0.56
1:A:406:GLN:HG2	8:A:872:HOH:O	2.05	0.56
1:A:312:VAL:HG11	1:A:332:ALA:HA	1.88	0.55
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.87	0.55
1:A:205:PHE:CE2	1:A:209:PHE:HZ	2.24	0.55
1:A:150:ARG:NH1	1:A:154:SER:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD23	1:A:384:LEU:O	2.06	0.55
1:A:306:LEU:HD23	1:A:306:LEU:C	2.27	0.55
1:A:35:PRO:C	1:A:37:CYS:H	2.10	0.55
1:A:151:ILE:HD11	1:A:529:PHE:CE2	2.42	0.55
1:A:119:VAL:HG12	5:A:751:BOG:H62	1.89	0.55
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.47	0.54
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.42	0.54
1:A:246:LEU:O	1:A:246:LEU:HG	2.07	0.54
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.73	0.54
1:A:275:TYR:HB2	1:A:284:GLN:OE1	2.07	0.54
1:A:289:GLN:HB3	1:A:292:PHE:CG	2.43	0.54
1:A:120:ARG:CZ	5:A:751:BOG:H1'1	2.37	0.54
1:A:137:ILE:N	1:A:137:ILE:HD12	2.23	0.54
1:A:75:TRP:CE3	1:A:78:LEU:HD12	2.43	0.53
1:A:245:ARG:HB2	1:A:247:PHE:CE1	2.43	0.53
1:A:204:HIS:HE2	1:A:232:HIS:CD2	2.27	0.53
1:A:114:ARG:HD3	1:A:365:LEU:O	2.08	0.53
1:A:402:TYR:HA	1:A:406:GLN:OE1	2.08	0.53
1:A:96:GLY:C	1:A:98:TRP:H	2.10	0.53
1:A:240:ARG:NH1	1:A:271:VAL:HG22	2.23	0.53
1:A:376:ARG:HH11	1:A:376:ARG:HB2	1.74	0.53
1:A:196:LEU:HD11	1:A:429:GLN:NE2	2.23	0.53
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.44	0.53
1:A:337:ILE:O	1:A:341:ILE:HG13	2.09	0.53
1:A:292:PHE:CD1	1:A:298:LEU:HD23	2.43	0.53
1:A:265:SER:HA	1:A:285:MET:HA	1.91	0.53
1:A:266:VAL:HG12	1:A:270:PRO:HA	1.91	0.53
1:A:287:VAL:HG23	1:A:288:GLY:N	2.24	0.52
1:A:145:VAL:O	1:A:145:VAL:CG1	2.57	0.52
1:A:478:PHE:CE1	1:A:498:ILE:HA	2.45	0.52
1:A:99:LEU:HD22	5:A:753:BOG:H1'2	1.91	0.52
1:A:204:HIS:NE2	1:A:232:HIS:CD2	2.77	0.52
1:A:242:TYR:CD2	1:A:247:PHE:CZ	2.97	0.52
1:A:295:LEU:HD21	1:A:408:LEU:CD2	2.40	0.52
1:A:291:VAL:HG23	1:A:294:LEU:HD12	1.92	0.51
1:A:526:GLY:HA3	7:A:700:ACD:H9	1.93	0.51
1:A:282:GLN:HA	1:A:282:GLN:NE2	2.26	0.51
1:A:254:TYR:CD1	1:A:261:VAL:HG13	2.46	0.51
1:A:267:GLU:O	1:A:268:GLU:HB2	2.10	0.51
1:A:376:ARG:HB2	1:A:376:ARG:NH1	2.26	0.51
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:N	1:A:281:PRO:CD	2.74	0.51
1:A:148:TYR:CE1	1:A:221:THR:HB	2.46	0.51
1:A:292:PHE:CE1	1:A:298:LEU:HD23	2.46	0.51
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.92	0.51
1:A:521:SER:O	1:A:525:MET:HB2	2.10	0.51
1:A:99:LEU:O	1:A:103:VAL:HG23	2.10	0.50
1:A:180:ARG:HD2	1:A:490:GLU:OE2	2.10	0.50
1:A:308:GLU:O	1:A:311:ARG:HB3	2.10	0.50
1:A:320:HIS:O	1:A:323:TRP:HB2	2.10	0.50
1:A:241:GLN:O	1:A:245:ARG:HG3	2.12	0.50
1:A:523:ILE:HG23	7:A:700:ACD:C5	2.42	0.50
1:A:574:THR:O	1:A:576:PRO:HD3	2.12	0.50
1:A:308:GLU:HG3	1:A:336:LEU:HD21	1.93	0.50
1:A:200:PHE:O	1:A:201:PHE:C	2.50	0.50
1:A:234:TYR:OH	1:A:336:LEU:HD12	2.12	0.50
1:A:295:LEU:HD21	1:A:408:LEU:HD23	1.94	0.50
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.50
1:A:245:ARG:NH2	1:A:325:ASP:OD2	2.45	0.50
1:A:408:LEU:O	1:A:410:ASN:N	2.45	0.50
1:A:279:ILE:HG22	1:A:279:ILE:O	2.11	0.49
1:A:238:LEU:HB3	1:A:239:GLU:OE2	2.12	0.49
1:A:409:PHE:C	1:A:410:ASN:O	2.49	0.49
1:A:181:PHE:HB3	1:A:509:LEU:HD21	1.94	0.49
1:A:409:PHE:O	1:A:410:ASN:C	2.48	0.49
1:A:294:LEU:O	1:A:295:LEU:HG	2.13	0.48
1:A:298:LEU:H	1:A:298:LEU:HD12	1.77	0.48
1:A:512:CYS:SG	1:A:518:PHE:HA	2.53	0.48
1:A:230:LEU:C	1:A:232:HIS:H	2.16	0.48
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.94	0.48
1:A:385:TYR:CE1	7:A:700:ACD:H131	2.47	0.48
1:A:363:PRO:HG2	1:A:545:TRP:CE2	2.48	0.48
1:A:99:LEU:CD2	5:A:753:BOG:H3'2	2.43	0.48
1:A:459:ARG:HG2	1:A:459:ARG:NH2	2.29	0.48
1:A:95:HIS:O	1:A:97:ARG:N	2.44	0.48
1:A:419:VAL:O	1:A:420:GLU:C	2.52	0.48
1:A:348:TYR:CE2	7:A:700:ACD:H12	2.32	0.48
1:A:115:LEU:HD13	5:A:752:BOG:H3'2	1.96	0.48
1:A:195:ASN:O	1:A:198:PHE:HB3	2.13	0.48
1:A:99:LEU:HD22	5:A:753:BOG:H3'2	1.95	0.48
1:A:74:ILE:CG2	1:A:75:TRP:N	2.76	0.48
1:A:226:HIS:HB3	1:A:377:ILE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:HIS:CD2	1:A:309:HIS:C	2.86	0.47
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.49	0.47
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.48	0.47
1:A:498:ILE:HG23	1:A:499:ASP:N	2.28	0.47
1:A:298:LEU:N	1:A:298:LEU:HD12	2.29	0.47
1:A:120:ARG:NH1	5:A:751:BOG:H1'1	2.29	0.47
1:A:91:PHE:HD2	1:A:92:LEU:HD12	1.79	0.47
1:A:201:PHE:C	1:A:201:PHE:CD2	2.88	0.47
1:A:206:THR:HA	1:A:209:PHE:CZ	2.50	0.47
1:A:404:TYR:CG	1:A:443:HIS:CD2	3.03	0.47
1:A:408:LEU:HB3	1:A:409:PHE:CE1	2.49	0.47
1:A:327:GLN:O	1:A:328:LEU:C	2.52	0.47
1:A:238:LEU:HG	1:A:242:TYR:CE1	2.49	0.47
1:A:433:ARG:HG2	1:A:433:ARG:NH1	2.28	0.47
1:A:165:THR:HG21	8:A:827:HOH:O	2.15	0.47
1:A:340:THR:O	1:A:344:VAL:HG23	2.15	0.47
1:A:251:LYS:HE3	8:A:880:HOH:O	2.14	0.46
1:A:137:ILE:HA	8:A:803:HOH:O	2.15	0.46
1:A:35:PRO:C	1:A:37:CYS:N	2.68	0.46
1:A:243:GLN:HG3	1:A:270:PRO:CG	2.41	0.46
1:A:279:ILE:N	1:A:280:PRO:HD3	2.30	0.46
1:A:517:ILE:HG23	1:A:518:PHE:CG	2.51	0.46
7:A:700:ACD:H71	7:A:700:ACD:H41	1.76	0.46
1:A:228:VAL:O	1:A:337:ILE:HG23	2.14	0.46
1:A:233:ILE:HD13	1:A:305:TRP:HB3	1.97	0.46
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.31	0.46
8:A:862:HOH:O	4:D:2:NAG:H2	2.16	0.46
1:A:360:LYS:HE2	1:A:362:ASP:CB	2.46	0.45
1:A:510:GLU:OE2	1:A:521:SER:N	2.45	0.45
1:A:294:LEU:C	1:A:295:LEU:HG	2.36	0.45
1:A:197:MET:SD	1:A:301:TYR:OH	2.74	0.45
1:A:275:TYR:OH	1:A:285:MET:N	2.47	0.45
1:A:530:SER:O	1:A:534:LEU:HD22	2.17	0.45
1:A:165:THR:CG2	8:A:827:HOH:O	2.64	0.45
1:A:204:HIS:CD2	1:A:232:HIS:HD2	2.35	0.45
1:A:389:PRO:HD3	1:A:440:ILE:HG12	1.98	0.45
1:A:35:PRO:O	1:A:37:CYS:N	2.49	0.45
1:A:239:GLU:CD	1:A:239:GLU:N	2.54	0.45
1:A:297:GLY:O	1:A:300:LEU:HB3	2.16	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.80	0.45
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CD1	1:A:580:PHE:HZ	2.34	0.45
1:A:282:GLN:CD	1:A:283:SER:H	2.19	0.45
1:A:183:LEU:HB2	1:A:445:LEU:HD22	1.98	0.45
1:A:246:LEU:HD12	1:A:253:LYS:HG2	1.99	0.45
1:A:449:VAL:O	1:A:453:LYS:HG3	2.18	0.45
1:A:462:PRO:O	1:A:463:PHE:C	2.55	0.44
1:A:157:ARG:NH1	1:A:459:ARG:HD2	2.32	0.44
1:A:239:GLU:OE2	1:A:239:GLU:N	2.46	0.44
1:A:323:TRP:CE3	1:A:328:LEU:HD23	2.45	0.44
1:A:335:ILE:O	1:A:339:GLU:HG3	2.17	0.44
1:A:523:ILE:HG23	7:A:700:ACD:C6	2.48	0.44
1:A:321:PRO:C	1:A:323:TRP:H	2.21	0.44
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.57	0.44
1:A:307:ARG:HG2	1:A:571:ASN:HB3	1.99	0.44
1:A:61:ARG:NH2	8:A:820:HOH:O	2.51	0.44
1:A:295:LEU:HB2	1:A:298:LEU:HD13	1.99	0.44
1:A:384:LEU:C	1:A:384:LEU:CD2	2.86	0.44
2:B:1:NAG:H61	2:B:2:NDG:C8	2.47	0.44
1:A:261:VAL:HB	1:A:307:ARG:HD3	1.99	0.44
1:A:279:ILE:C	1:A:281:PRO:HD3	2.35	0.44
1:A:292:PHE:O	1:A:299:MET:CE	2.66	0.44
1:A:357:LEU:HD12	1:A:358:GLN:N	2.32	0.44
1:A:444:ILE:O	1:A:446:HIS:N	2.51	0.44
1:A:395:PHE:N	1:A:395:PHE:CD1	2.86	0.44
1:A:120:ARG:HA	1:A:120:ARG:HD2	1.80	0.43
1:A:156:PRO:C	1:A:158:ASP:H	2.21	0.43
1:A:240:ARG:HD2	8:A:824:HOH:O	2.18	0.43
1:A:269:ALA:O	1:A:271:VAL:N	2.50	0.43
1:A:287:VAL:HG21	1:A:292:PHE:HB2	2.01	0.43
1:A:40:PRO:HG2	1:A:41:CYS:H	1.84	0.43
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.54	0.43
1:A:40:PRO:HG3	1:A:55:TYR:CE1	2.53	0.43
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.54	0.43
1:A:305:TRP:O	1:A:308:GLU:HB3	2.19	0.43
1:A:349:VAL:CG1	7:A:700:ACD:H42	2.47	0.43
1:A:145:VAL:O	1:A:145:VAL:HG12	2.19	0.43
1:A:158:ASP:N	1:A:158:ASP:OD1	2.51	0.43
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.65	0.43
1:A:208:GLN:NE2	1:A:230:LEU:N	2.59	0.43
1:A:445:LEU:HG	1:A:445:LEU:O	2.18	0.43
1:A:201:PHE:HD2	1:A:201:PHE:C	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA3	1:A:54:ARG:HH21	1.84	0.42
2:B:1:NAG:H61	2:B:2:NDG:H8C3	2.01	0.42
1:A:216:MET:HG2	3:C:2:NAG:C8	2.49	0.42
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.54	0.42
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.88	0.42
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.85	0.42
1:A:100:TRP:O	1:A:104:ASN:HB2	2.19	0.42
1:A:71:ILE:HA	1:A:72:PRO:HD2	1.81	0.42
1:A:131:ASN:OD1	1:A:134:HIS:N	2.49	0.42
1:A:517:ILE:HG23	1:A:518:PHE:CD1	2.55	0.42
1:A:137:ILE:H	1:A:137:ILE:HD12	1.84	0.42
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.59	0.42
1:A:467:ARG:HB3	1:A:467:ARG:HE	1.70	0.42
1:A:168:LYS:C	1:A:170:GLN:H	2.23	0.42
1:A:527:ALA:HB2	7:A:700:ACD:H22	2.02	0.42
1:A:157:ARG:HA	1:A:459:ARG:NH1	2.35	0.41
1:A:408:LEU:C	1:A:410:ASN:H	2.23	0.41
1:A:414:LEU:O	1:A:414:LEU:HD12	2.20	0.41
1:A:255:GLN:HG2	1:A:263:PRO:O	2.20	0.41
1:A:40:PRO:O	1:A:68:ASN:HB3	2.20	0.41
1:A:184:ARG:HB2	1:A:439:ASN:C	2.41	0.41
1:A:257:LEU:O	1:A:258:ASN:CB	2.67	0.41
1:A:282:GLN:CG	1:A:283:SER:N	2.83	0.41
1:A:362:ASP:HB3	1:A:365:LEU:HG	2.02	0.41
1:A:299:MET:HG3	1:A:414:LEU:CD2	2.50	0.41
1:A:125:PRO:HG2	8:A:818:HOH:O	2.20	0.41
1:A:391:MET:HG3	6:A:601:COH:HAB	2.03	0.41
1:A:280:PRO:HA	1:A:284:GLN:HG3	2.03	0.41
1:A:357:LEU:HD12	1:A:358:GLN:H	1.86	0.41
1:A:64:TYR:CZ	1:A:76:THR:HG21	2.55	0.41
1:A:204:HIS:ND1	1:A:301:TYR:HB3	2.36	0.41
1:A:280:PRO:HA	1:A:284:GLN:CD	2.41	0.41
1:A:392:PRO:HB3	1:A:429:GLN:HE21	1.86	0.41
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.86	0.41
1:A:187:PHE:CE1	1:A:189:PRO:HB3	2.56	0.40
1:A:199:ALA:HB1	1:A:391:MET:CE	2.50	0.40
1:A:168:LYS:C	1:A:170:GLN:N	2.74	0.40
1:A:145:VAL:HG11	1:A:224:LEU:HB3	2.03	0.40
1:A:171:LEU:HB3	1:A:456:ARG:HH21	1.86	0.40
1:A:256:MET:SD	1:A:261:VAL:HG22	2.61	0.40
1:A:152:LEU:C	1:A:153:PRO:O	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.56	0.40
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.79	0.40
1:A:582:VAL:HG22	1:A:583:PRO:N	2.36	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	551/553 (100%)	439 (80%)	90 (16%)	22 (4%)	<b>3</b> <b>17</b>

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	247	PHE
1	A	281	PRO
1	A	117	LEU
1	A	268	GLU
1	A	290	GLU
1	A	322	THR
1	A	409	PHE
1	A	551	GLY
1	A	569	CYS
1	A	157	ARG
1	A	277	ARG
1	A	36	CYS
1	A	118	THR
1	A	160	PRO
1	A	278	GLY
1	A	486	GLU
1	A	96	GLY

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Mol	Chain	Res	Type
1	A	270	PRO
1	A	145	VAL
1	A	116	VAL
1	A	153	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	468/488 (96%)	432 (92%)	36 (8%)	13	42

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	80	THR
1	A	97	ARG
1	A	99	LEU
1	A	106	THR
1	A	120	ARG
1	A	136	TYR
1	A	180	ARG
1	A	185	ARG
1	A	201	PHE
1	A	209	PHE
1	A	228	VAL
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	289	GLN
1	A	326	GLU
1	A	375	ASN
1	A	376	ARG

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	385	TYR
1	A	414	LEU
1	A	442	HIS
1	A	484	GLU
1	A	518	PHE
1	A	530	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	56	GLN
1	A	203	GLN
1	A	208	GLN
1	A	232	HIS
1	A	237	ASN
1	A	241	GLN
1	A	258	ASN
1	A	282	GLN
1	A	375	ASN
1	A	443	HIS
1	A	557	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 ⓘ

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	0.69	0	17,19,21	1.11	2 (11%)
2	NDG	B	2	2	14,14,15	0.61	0	17,19,21	1.45	3 (17%)
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	0.97	2 (11%)
3	NAG	C	2	3	14,14,15	0.92	0	17,19,21	1.57	3 (17%)
3	BMA	C	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.46	2 (13%)
3	BMA	C	4	3	11,11,12	1.09	0	15,15,17	1.21	2 (13%)
3	MAN	C	5	3	11,11,12	0.78	0	15,15,17	0.79	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.57	0	17,19,21	0.80	1 (5%)
4	NAG	D	2	4	14,14,15	0.61	0	17,19,21	1.31	2 (11%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	2.52	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-C2-C3	4.41	115.09	109.67
3	C	2	NAG	C4-C3-C2	-4.30	104.72	111.02
4	D	2	NAG	C2-N2-C7	-3.70	117.64	122.90
2	B	2	NDG	C4-C3-C2	3.66	116.39	111.02
3	C	4	BMA	C1-O5-C5	3.54	116.99	112.19
3	C	2	NAG	C1-C2-N2	3.01	115.63	110.49
4	D	2	NAG	C4-C3-C2	-2.84	106.85	111.02
2	B	2	NDG	C3-C4-C5	2.78	115.19	110.24
2	B	1	NAG	C2-N2-C7	-2.77	118.96	122.90
2	B	2	NDG	C2-N2-C7	-2.45	119.42	122.90
3	C	2	NAG	O5-C1-C2	-2.41	107.48	111.29
3	C	3	BMA	C1-O5-C5	2.39	115.43	112.19
3	C	4	BMA	O3-C3-C2	2.34	114.47	109.99
3	C	5	MAN	C1-O5-C5	2.28	115.28	112.19
2	B	1	NAG	C4-C3-C2	-2.27	107.69	111.02
3	C	1	NAG	C2-N2-C7	-2.15	119.84	122.90
4	D	1	NAG	C2-N2-C7	-2.03	120.01	122.90
3	C	1	NAG	C1-O5-C5	2.02	114.94	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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

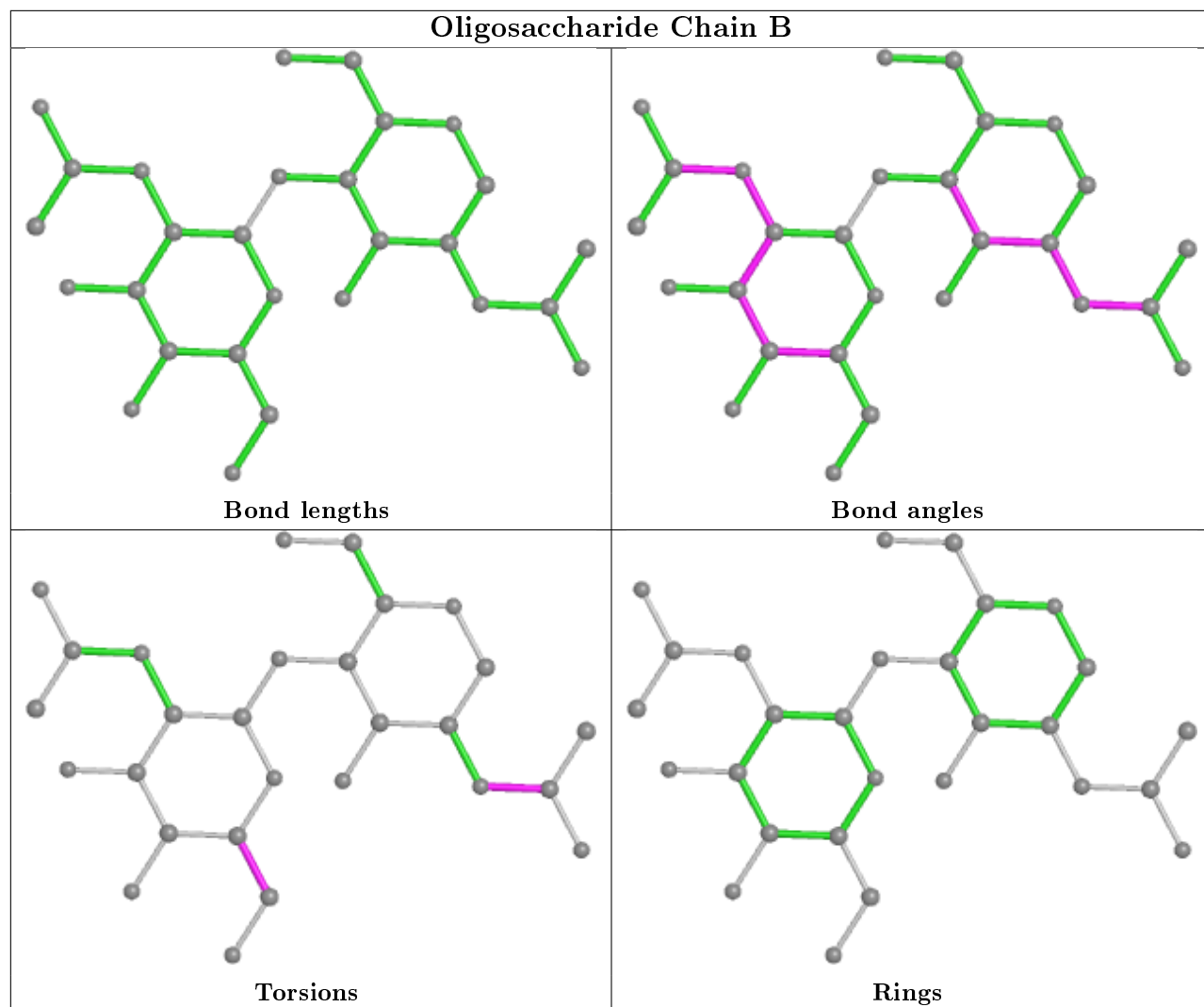
All (2) ring outliers are listed below:

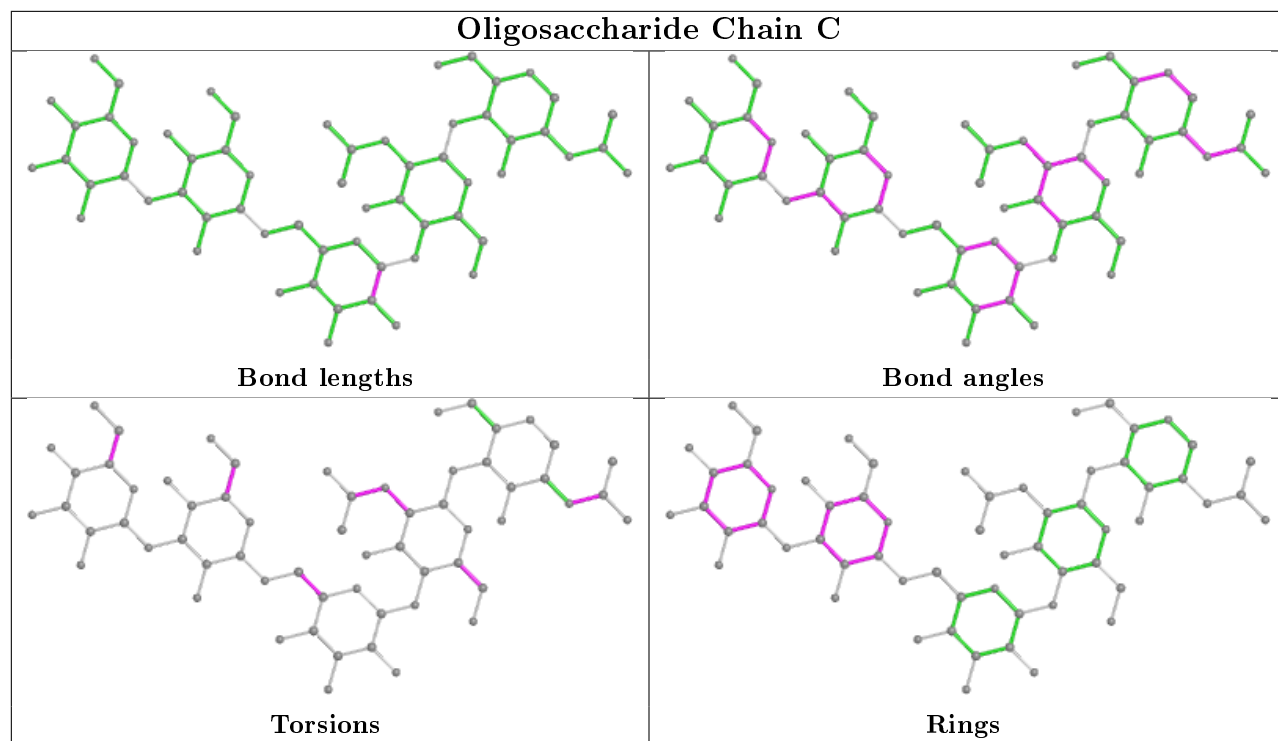
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	C1-C2-C3-C4-C5-O5
3	C	4	BMA	C1-C2-C3-C4-C5-O5

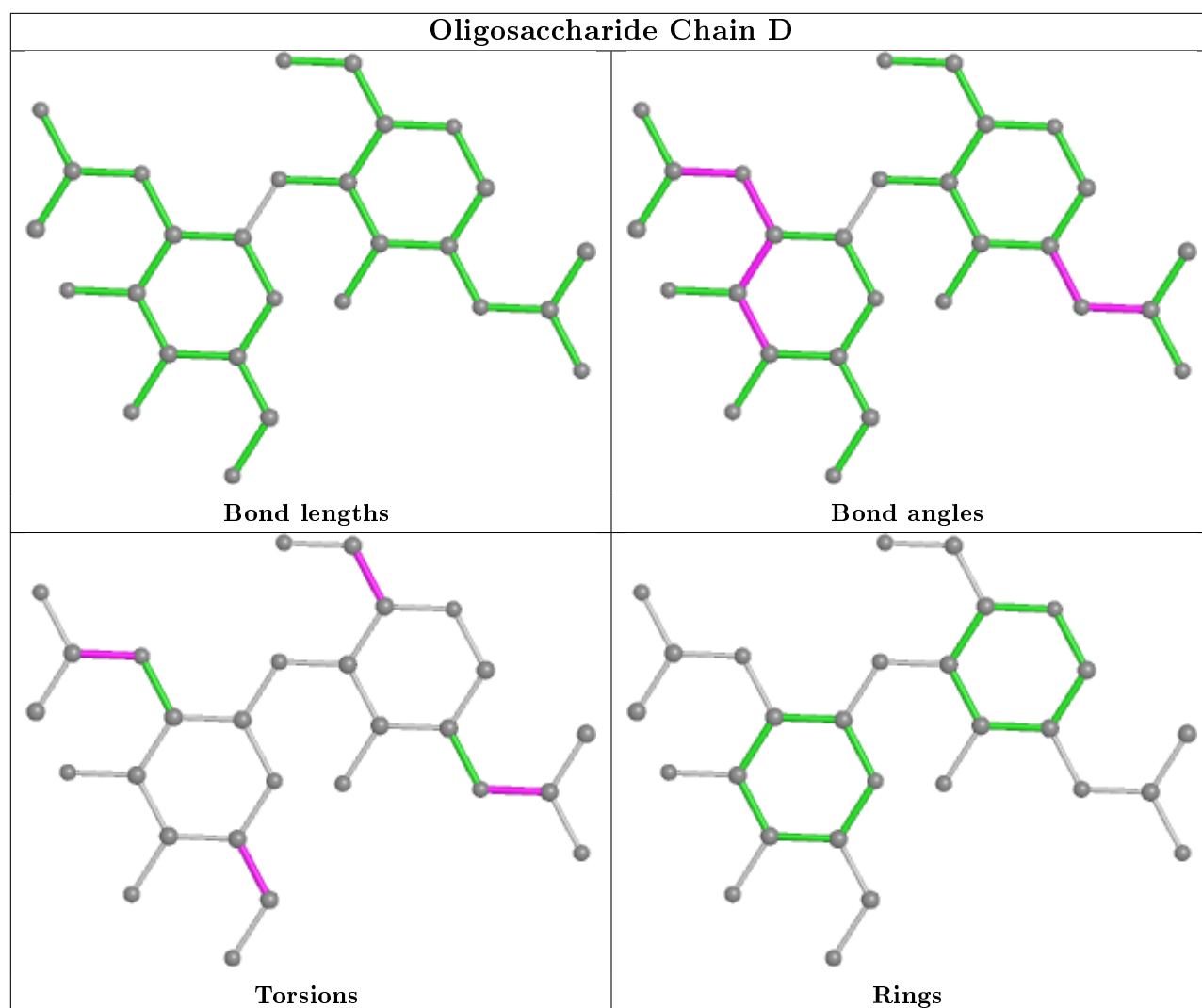
4 monomers are involved in 5 short contacts:

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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	ACD	A	700	-	18,21,21	0.63	0	17,21,21	0.87	0
5	BOG	A	750	-	20,20,20	0.44	0	25,25,25	0.63	1 (4%)
5	BOG	A	753	-	20,20,20	0.74	0	25,25,25	0.89	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BOG	A	751	-	20,20,20	0.50	0	25,25,25	0.78	1 (4%)
5	BOG	A	752	-	20,20,20	0.59	0	25,25,25	0.88	2 (8%)
6	COH	A	601	1	31,50,50	7.20	21 (67%)	23,82,82	4.67	11 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ACD	A	700	-	-	5/17/19/19	-
5	BOG	A	750	-	-	3/11/31/31	0/1/1/1
5	BOG	A	753	-	-	4/11/31/31	0/1/1/1
5	BOG	A	751	-	-	7/11/31/31	0/1/1/1
5	BOG	A	752	-	-	5/11/31/31	0/1/1/1
6	COH	A	601	1	-	2/8/94/94	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	COH	C4D-ND	18.50	1.44	1.34
6	A	601	COH	C1D-C2D	13.21	1.56	1.38
6	A	601	COH	C1B-NB	12.97	1.41	1.34
6	A	601	COH	C4B-NB	11.72	1.40	1.34
6	A	601	COH	C3A-C2A	11.66	1.43	1.34
6	A	601	COH	CHB-C4A	-10.91	1.34	1.53
6	A	601	COH	CHD-C4C	-9.11	1.37	1.53
6	A	601	COH	CHC-C1C	-8.55	1.38	1.53
6	A	601	COH	CHA-C1A	-7.61	1.40	1.53
6	A	601	COH	C1B-C2B	7.18	1.47	1.38
6	A	601	COH	CAA-C2A	6.42	1.60	1.51
6	A	601	COH	C4C-C3C	-5.92	1.42	1.51
6	A	601	COH	CHB-C1B	-5.87	1.36	1.51
6	A	601	COH	CHA-C4D	-5.29	1.38	1.51
6	A	601	COH	C4D-C3D	5.22	1.45	1.38
6	A	601	COH	CHC-C4B	-5.07	1.38	1.51
6	A	601	COH	CMC-C2C	4.35	1.57	1.50
6	A	601	COH	CHD-C1D	-3.69	1.42	1.51
6	A	601	COH	CAD-C3D	3.14	1.56	1.52
6	A	601	COH	CBC-CAC	2.89	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	COH	C3B-C2B	-2.70	1.36	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	COH	CHC-C1C-NC	10.51	125.59	110.12
6	A	601	COH	CHB-C4A-NA	9.24	123.72	110.12
6	A	601	COH	CHA-C1A-NA	8.35	122.41	110.12
6	A	601	COH	CHD-C4C-NC	8.26	122.28	110.12
6	A	601	COH	C3C-C4C-NC	7.01	114.43	109.03
6	A	601	COH	CAD-C3D-C4D	-6.51	122.72	127.30
6	A	601	COH	CMD-C2D-C3D	4.76	133.92	124.94
6	A	601	COH	CHC-C4B-C3B	-3.46	124.90	129.55
6	A	601	COH	CHB-C1B-C2B	-3.17	123.96	129.45
5	A	752	BOG	C1'-O1-C1	3.15	119.06	113.84
5	A	753	BOG	C1'-O1-C1	2.86	118.58	113.84
6	A	601	COH	CHD-C1D-C2D	-2.59	124.97	129.45
6	A	601	COH	C3D-C4D-ND	2.52	112.58	109.94
5	A	751	BOG	C1'-O1-C1	2.44	117.89	113.84
5	A	752	BOG	O1-C1-C2	2.26	111.84	108.30
5	A	750	BOG	C1'-O1-C1	2.09	117.31	113.84

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	700	ACD	C12-C13-C14-C15
5	A	750	BOG	C2'-C1'-O1-C1
5	A	753	BOG	C2-C1-O1-C1'
5	A	753	BOG	O5-C1-O1-C1'
5	A	751	BOG	O5-C1-O1-C1'
5	A	752	BOG	C2-C1-O1-C1'
5	A	750	BOG	O5-C5-C6-O6
5	A	750	BOG	C4-C5-C6-O6
5	A	752	BOG	O5-C5-C6-O6
5	A	752	BOG	C4-C5-C6-O6
5	A	753	BOG	O5-C5-C6-O6
6	A	601	COH	C2C-C3C-CAC-CBC
5	A	751	BOG	C2-C1-O1-C1'
7	A	700	ACD	C5-C6-C7-C8
7	A	700	ACD	C6-C7-C8-C9
7	A	700	ACD	C9-C10-C11-C12

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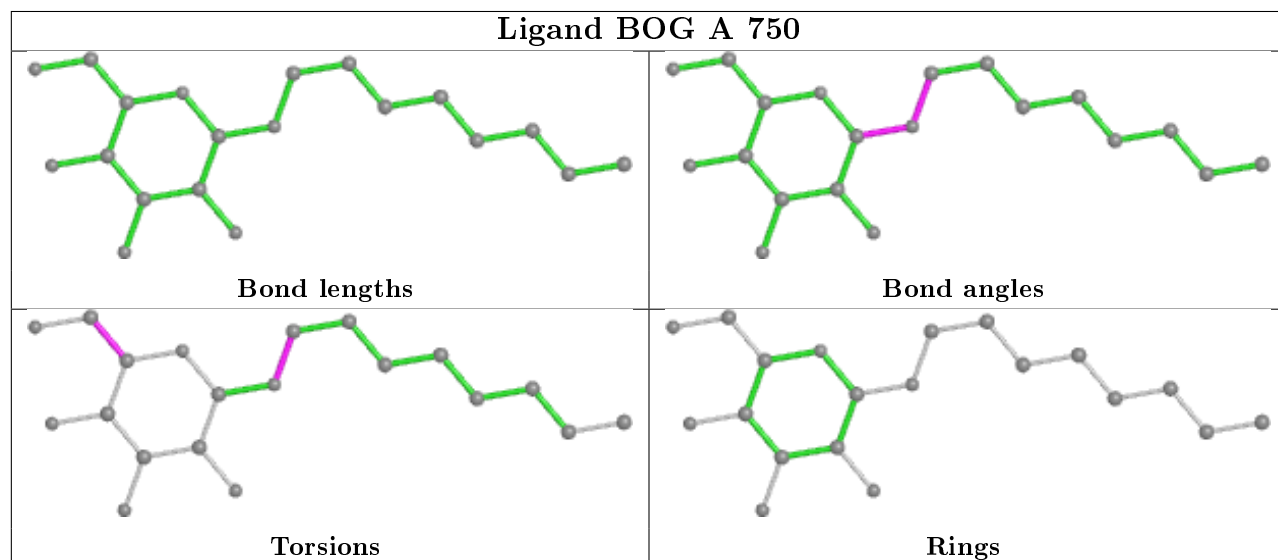
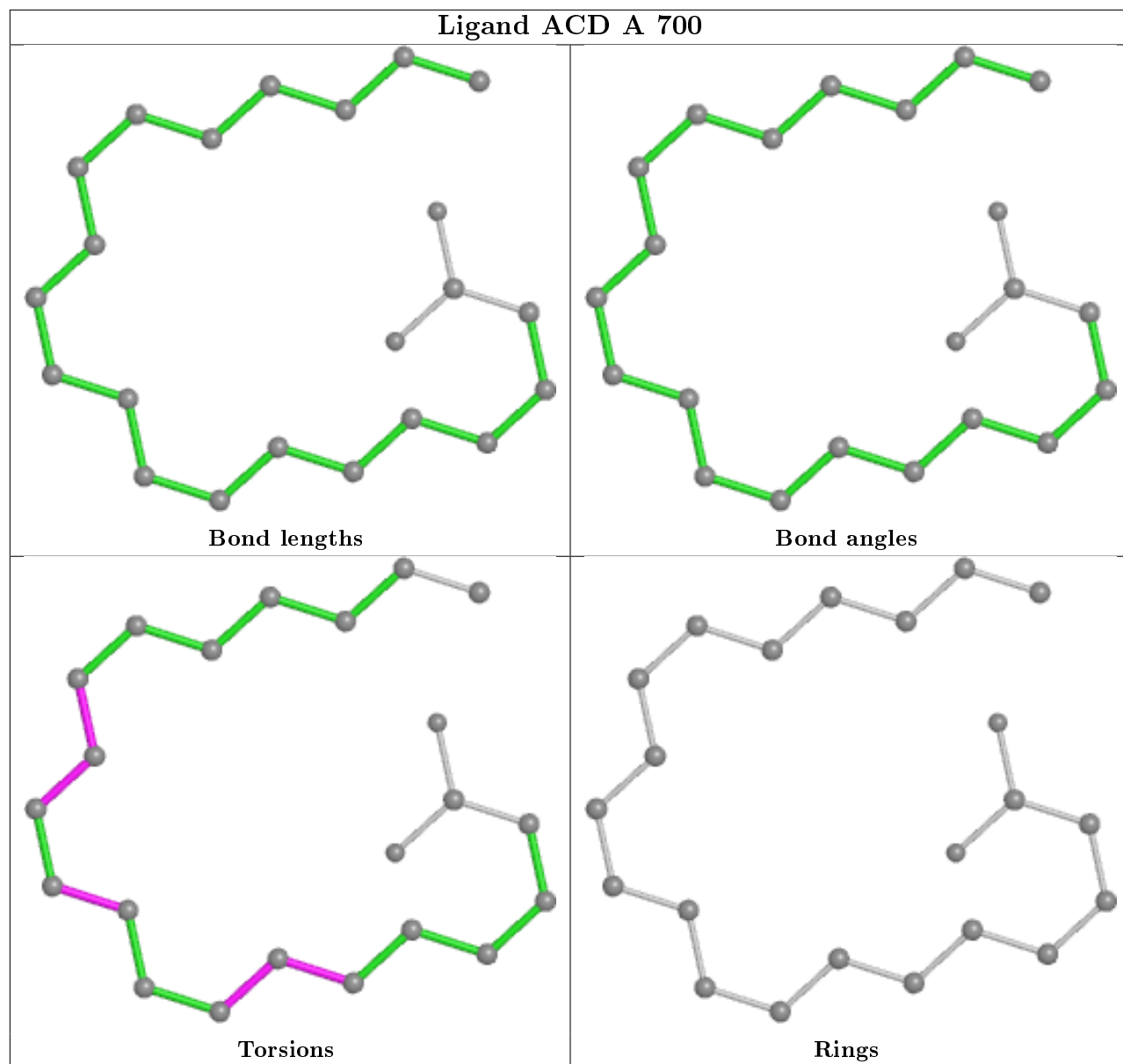
Mol	Chain	Res	Type	Atoms
5	A	751	BOG	C1'-C2'-C3'-C4'
6	A	601	COH	C4C-C3C-CAC-CBC
5	A	752	BOG	O5-C1-O1-C1'
5	A	751	BOG	C4-C5-C6-O6
5	A	751	BOG	C4'-C5'-C6'-C7'
5	A	753	BOG	C4-C5-C6-O6
7	A	700	ACD	C11-C12-C13-C14
5	A	752	BOG	C3'-C4'-C5'-C6'
5	A	751	BOG	C2'-C1'-O1-C1
5	A	751	BOG	O5-C5-C6-O6

There are no ring outliers.

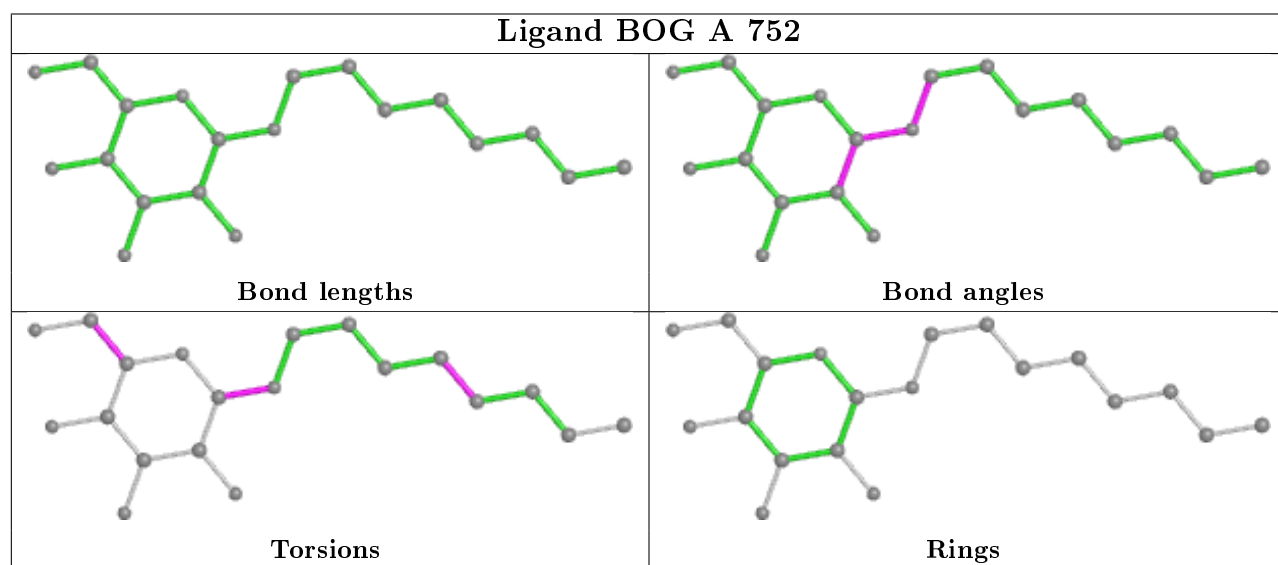
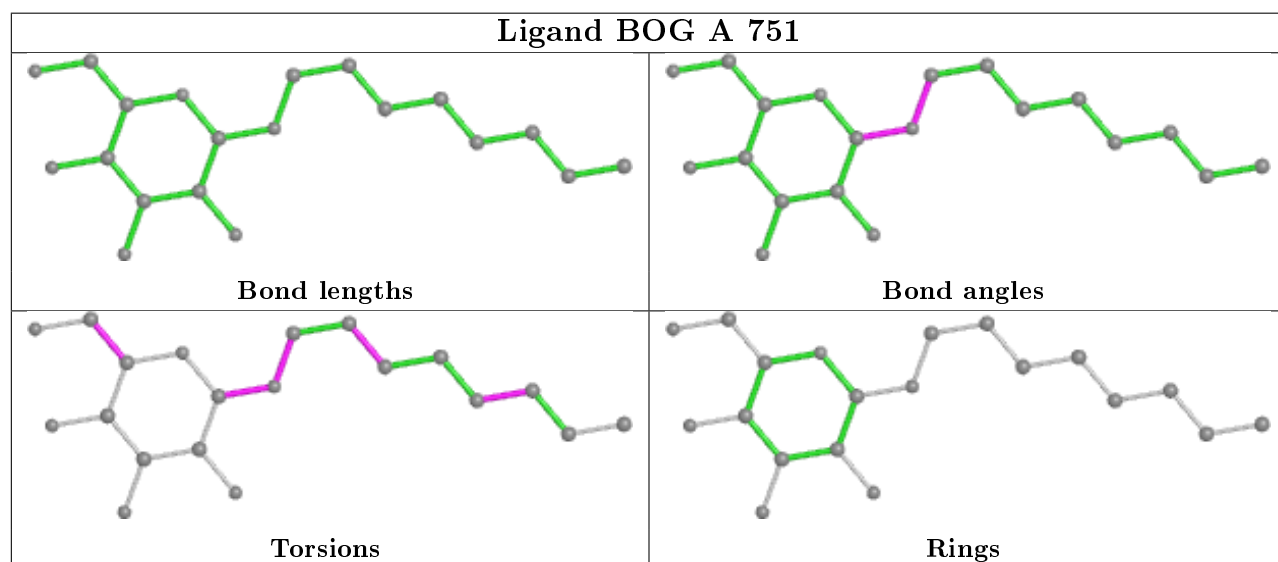
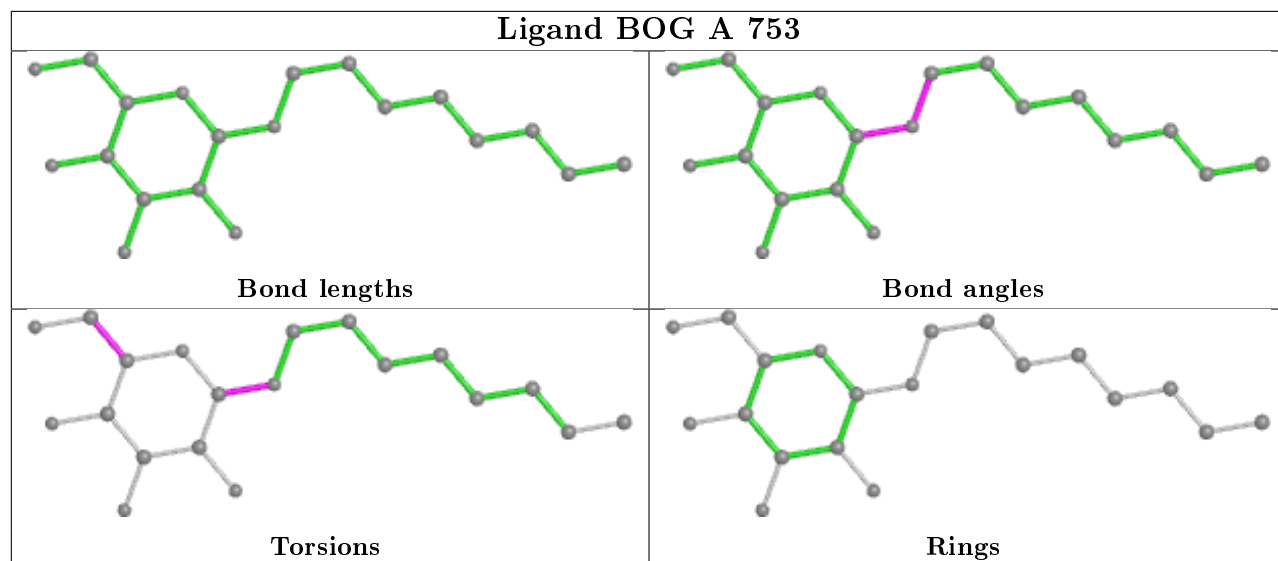
5 monomers are involved in 25 short contacts:

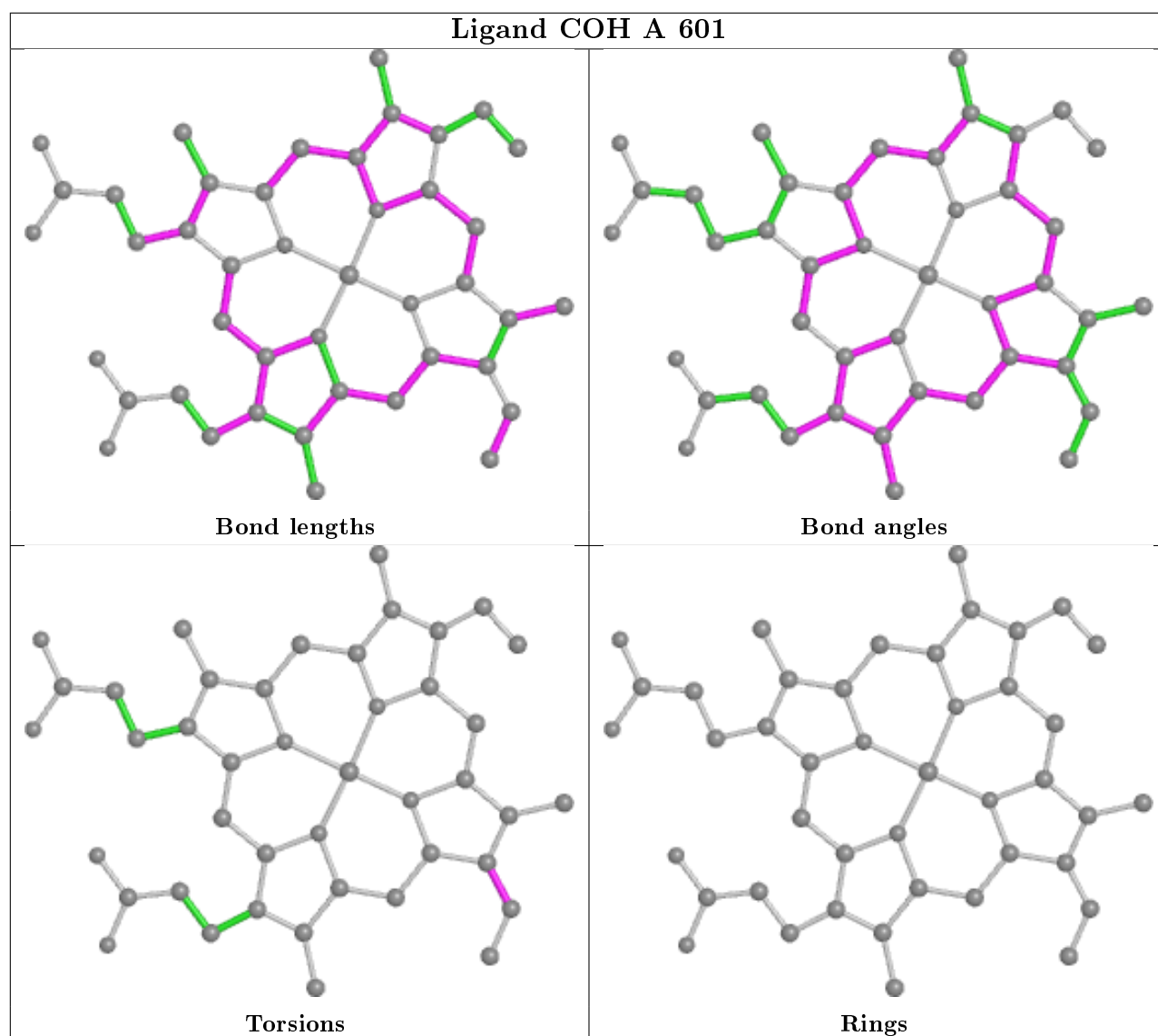
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	700	ACD	13	0
5	A	753	BOG	5	0
5	A	751	BOG	5	0
5	A	752	BOG	1	0
6	A	601	COH	1	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	553/553 (100%)	-0.78	0 100 100	21, 44, 65, 111	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

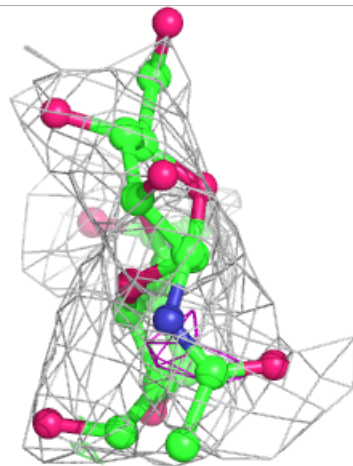
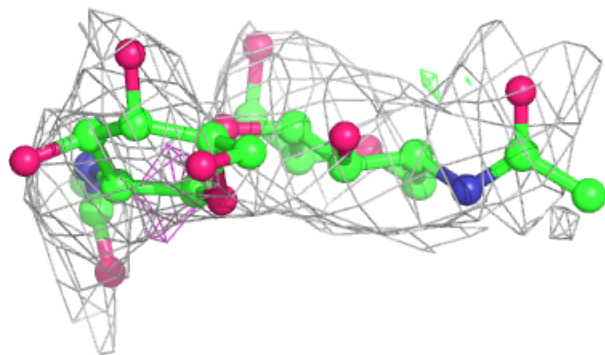
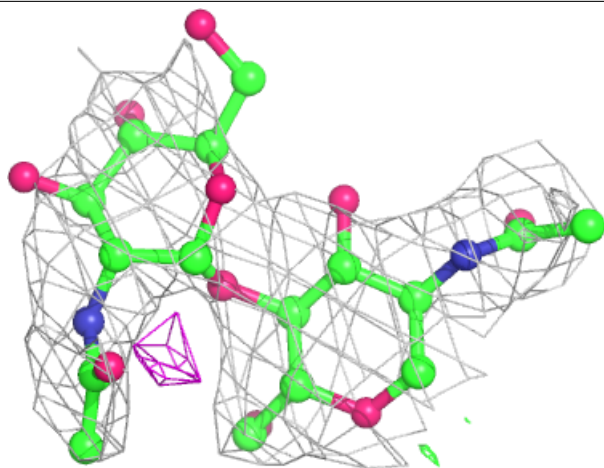
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	C	4	11/12	0.78	0.29	81,81,81,81	0
3	MAN	C	5	11/12	0.83	0.27	78,78,78,78	0
2	NDG	B	2	14/15	0.84	0.31	71,71,71,71	0
2	NAG	B	1	14/15	0.85	0.23	71,71,71,71	0
4	NAG	D	2	14/15	0.85	0.25	63,63,63,63	0
3	NAG	C	1	14/15	0.88	0.19	42,42,42,42	0
3	NAG	C	2	14/15	0.89	0.21	53,53,53,53	0
3	BMA	C	3	11/12	0.93	0.19	67,67,67,67	0
4	NAG	D	1	14/15	0.96	0.12	49,49,49,49	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

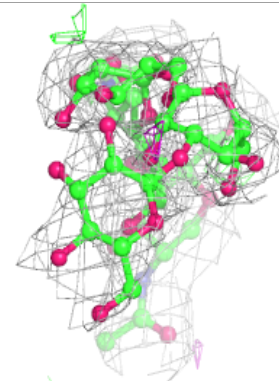
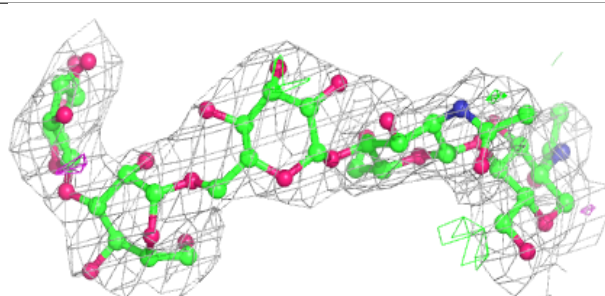
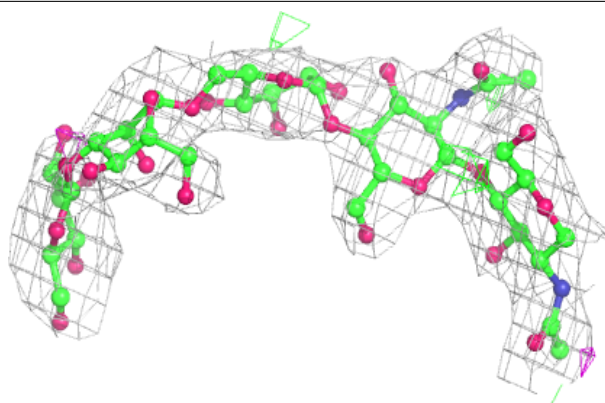
**Electron density around Chain B:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

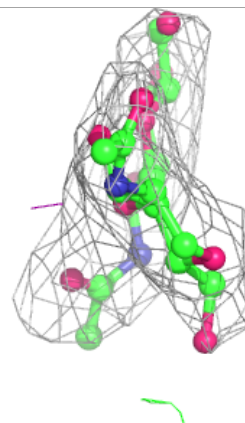
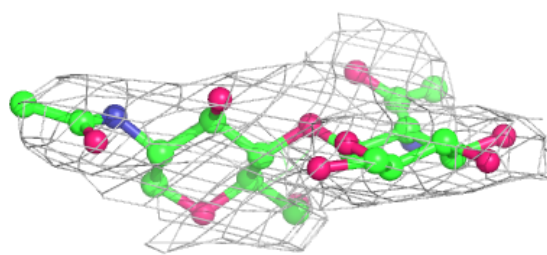
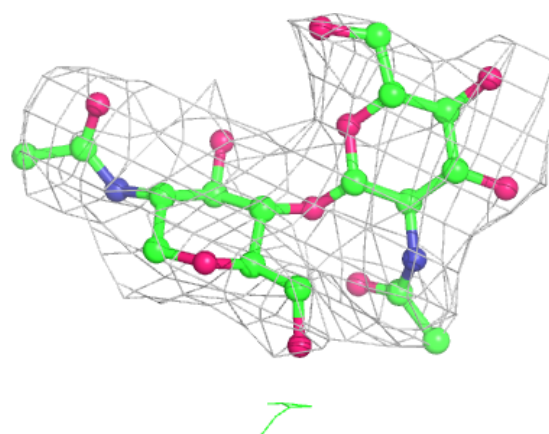


**Electron density around Chain C:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

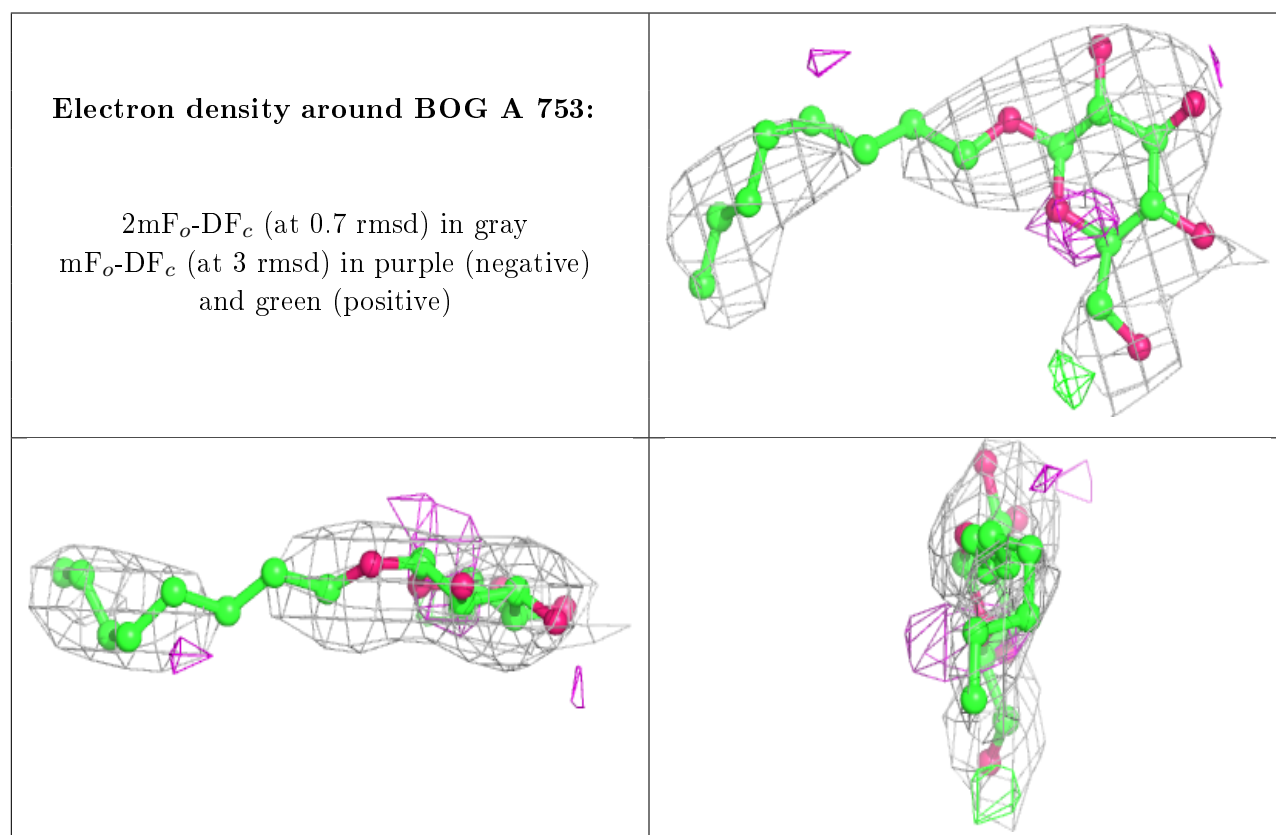


## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

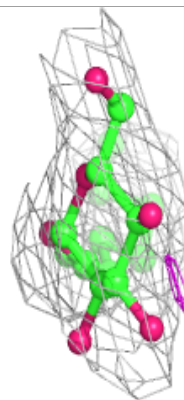
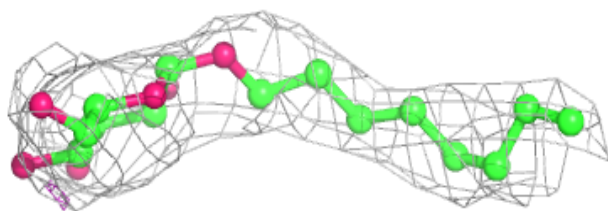
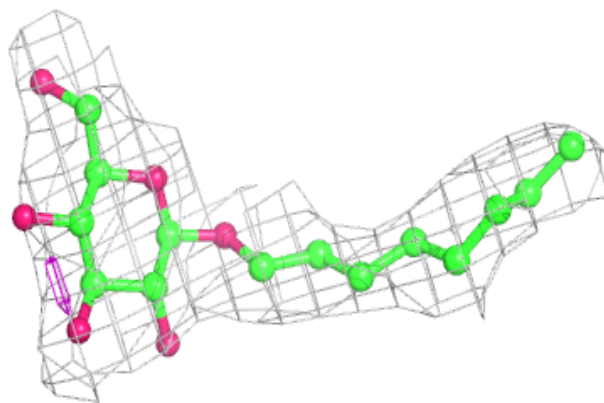
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BOG	A	753	20/20	0.72	0.35	86,86,86,86	0
5	BOG	A	752	20/20	0.86	0.22	78,78,78,78	0
6	COH	A	601	43/43	0.87	0.23	74,74,74,74	0
5	BOG	A	750	20/20	0.89	0.23	59,59,59,59	0
5	BOG	A	751	20/20	0.90	0.19	64,64,64,64	0
7	ACD	A	700	22/22	0.95	0.13	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



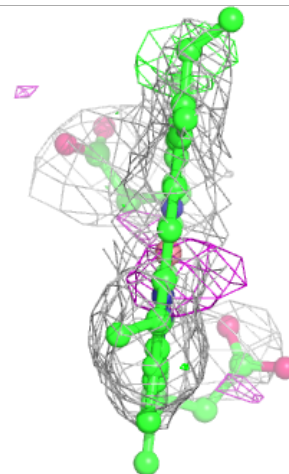
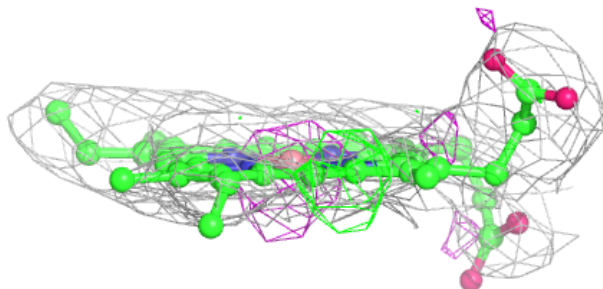
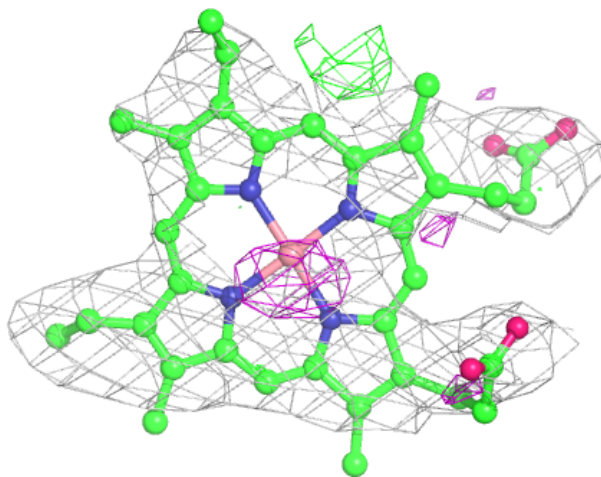
**Electron density around BOG A 752:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around COH A 601:**

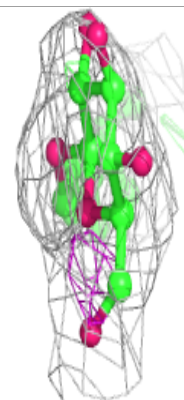
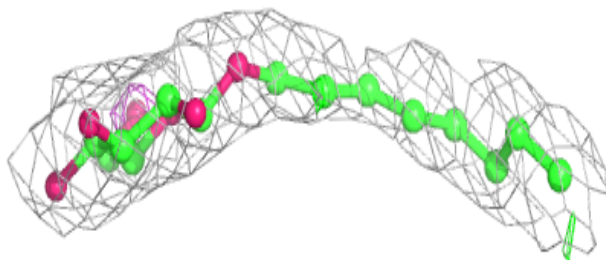
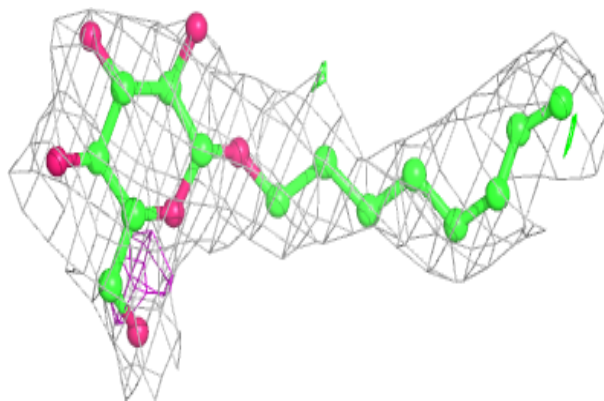
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



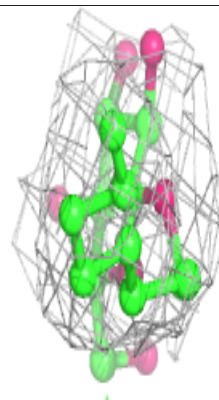
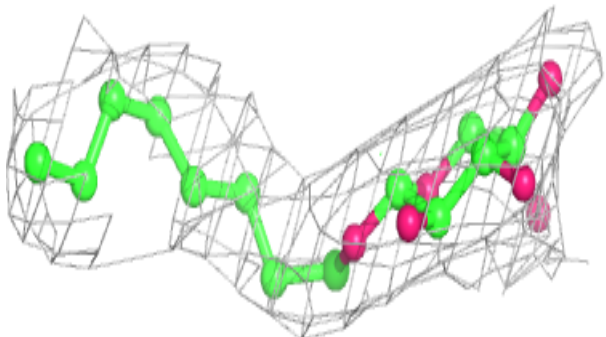
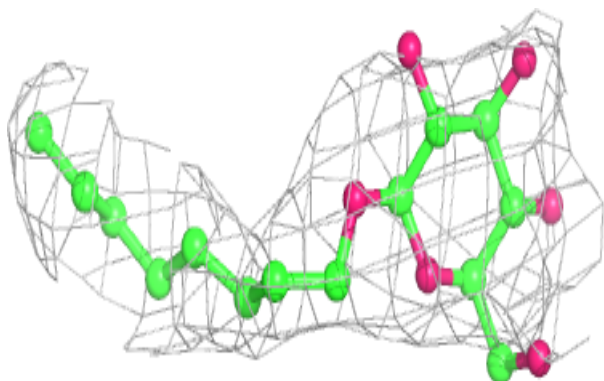


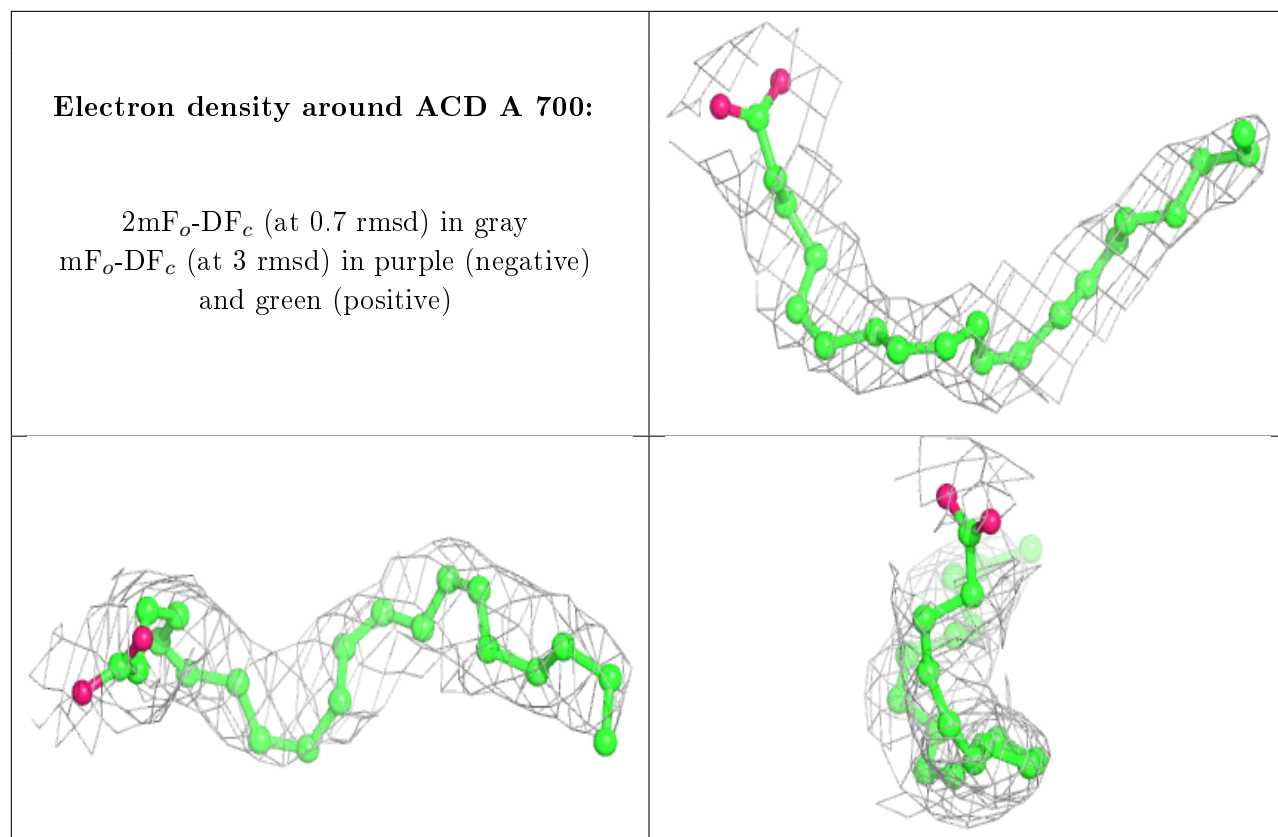
**Electron density around BOG A 750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BOG A 751:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.