



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:50 PM UTC

PDB ID : 1U67 / pdb_00001u67
Title : Crystal Structure of Arachidonic Acid Bound to a Mutant of Prostaglandin H Synthase-1 that Forms Predominantly 11-HPETE.
Authors : Harman, C.A.; Rieke, C.J.; Garavito, R.M.; Smith, W.L.
Deposited on : 2004-07-29
Resolution : 3.10 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

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>.

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)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

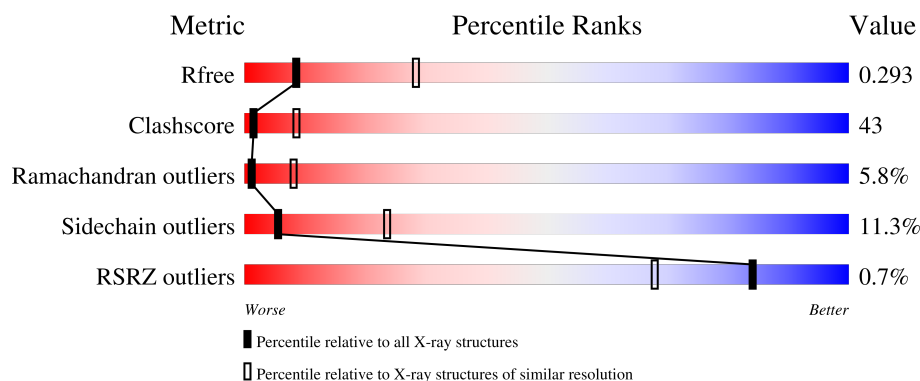
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 ≥ 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	600	31% 49% 11% 8%
2	B	2	100%
2	D	2	50% 50%
3	C	4	25% 50% 25%

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
4	BOG	A	753	-	-	-	X
5	COH	A	601	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4575 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 G/H synthase 1 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4307	2798	723	758	28			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	see remark 999	UNP P05979
A	349	ALA	VAL	engineered mutation	UNP P05979
A	387	PHE	TRP	engineered mutation	UNP P05979

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



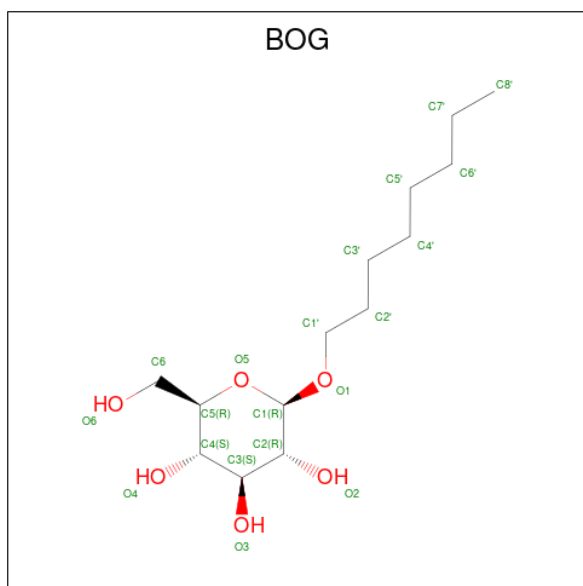
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 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.



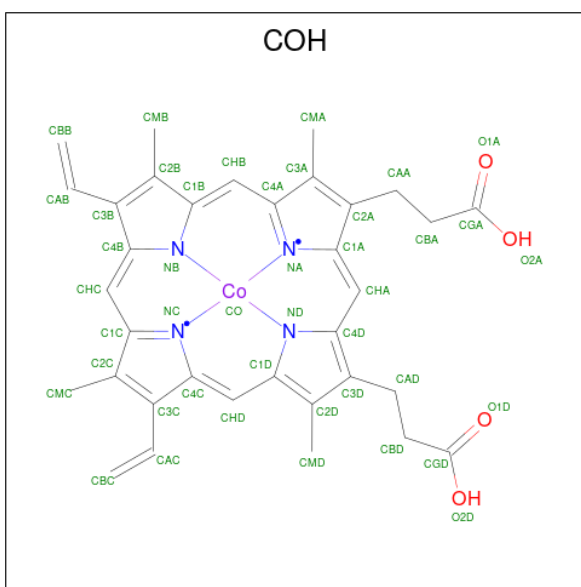
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



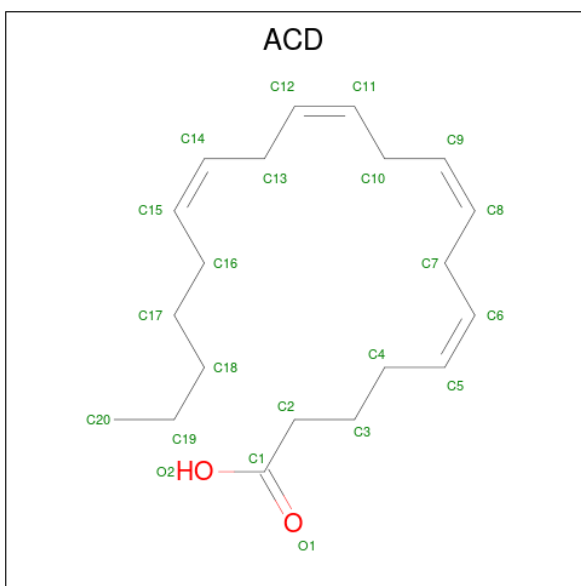
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



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

- Molecule 6 is ARACHIDONIC ACID (CCD ID: ACD) (formula: $\text{C}_{20}\text{H}_{32}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	13	2		

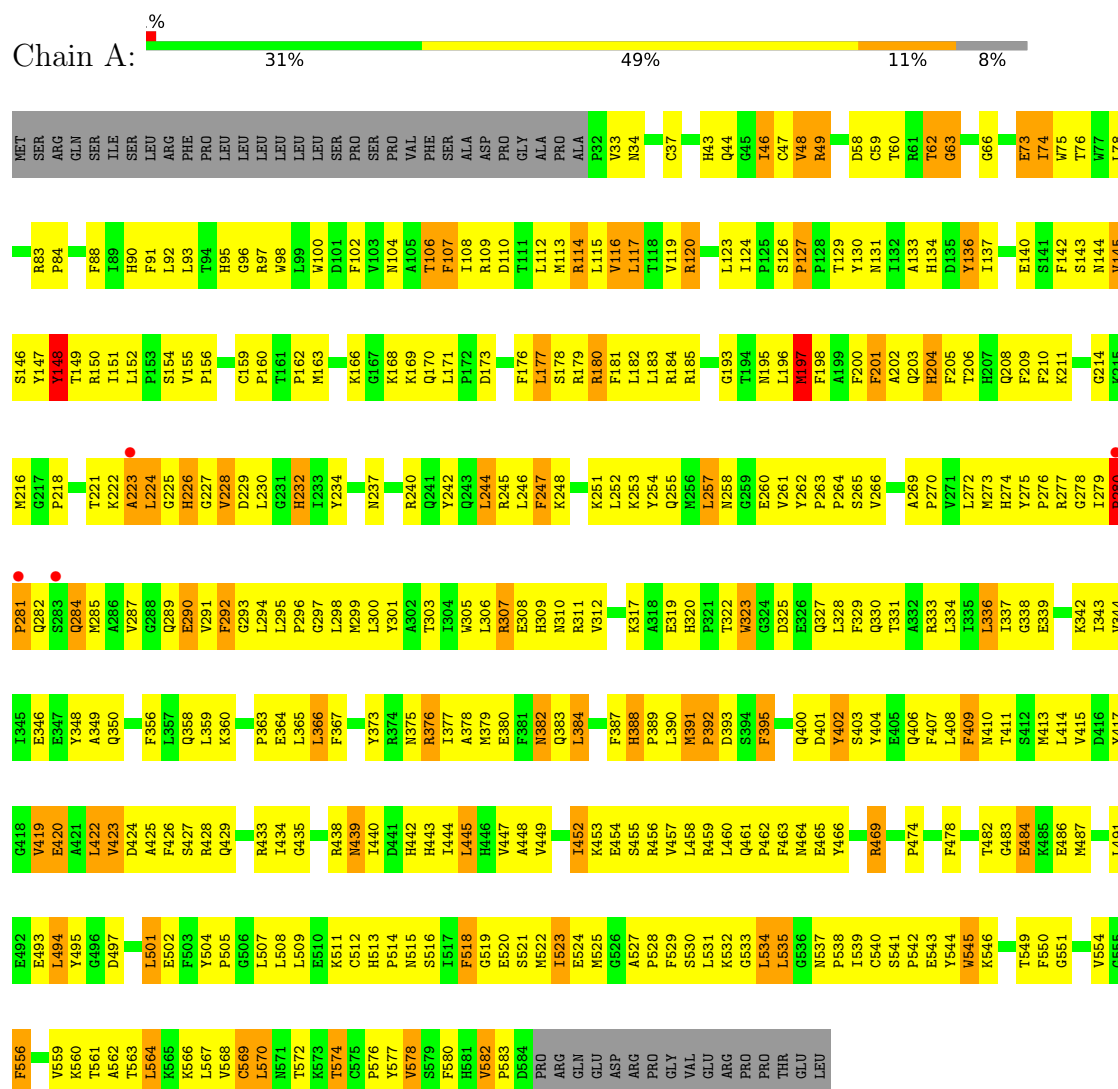
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total 24	O 24	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 G/H synthase 1 precursor



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



NAG1
NDG2

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

Chain D:  50% 50%

NAG1
NDG2

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

Chain C:  25% 50% 25%

NAG1
NAG2
BMA3
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.88Å 181.88Å 103.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-3.10) 94.3 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.55 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.311 0.230 , 0.293	Depositor DCC
R_{free} test set	810 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, NDG, ACD, COH, BOG, BMA

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	0.52	0/4445	1.06	29/6060 (0.5%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-9.44	96.90	110.59
1	A	423	VAL	N-CA-C	-8.29	103.74	111.45
1	A	129	THR	N-CA-C	8.04	123.14	112.13
1	A	564	LEU	N-CA-C	-7.81	101.87	111.40
1	A	232	HIS	N-CA-C	-7.66	100.98	112.54
1	A	63	GLY	N-CA-C	-7.46	104.75	115.27
1	A	287	VAL	N-CA-C	7.06	118.05	112.12
1	A	73	GLU	N-CA-C	-6.53	101.73	110.55
1	A	393	ASP	N-CA-C	-6.28	104.33	112.68
1	A	62	THR	N-CA-C	-6.27	104.44	111.28
1	A	280	PRO	N-CA-C	6.12	118.17	110.70
1	A	95	HIS	N-CA-C	6.12	121.60	114.62
1	A	214	GLY	N-CA-C	-6.01	106.89	114.16
1	A	66	GLY	CA-C-N	6.00	125.48	119.24
1	A	66	GLY	C-N-CA	6.00	125.48	119.24
1	A	356	PHE	N-CA-C	-5.91	106.22	113.50
1	A	402	TYR	N-CA-C	5.90	118.89	110.10
1	A	224	LEU	N-CA-C	-5.70	103.12	110.19
1	A	143	SER	N-CA-C	5.62	120.19	113.23
1	A	413	MET	N-CA-C	5.54	117.76	111.11
1	A	388	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
1	A	391	MET	CA-C-N	5.42	126.62	119.84
1	A	391	MET	C-N-CA	5.42	126.62	119.84
1	A	90	HIS	N-CA-C	-5.40	105.29	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	MET	N-CA-C	-5.33	105.58	111.71
1	A	346	GLU	N-CA-C	5.29	119.22	112.87
1	A	127	PRO	CA-C-N	5.27	125.55	119.92
1	A	127	PRO	C-N-CA	5.27	125.55	119.92
1	A	323	TRP	N-CA-C	5.15	117.81	110.24

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	4307	0	4015	378	0
2	B	28	0	24	1	0
2	D	28	0	24	0	0
3	C	50	0	43	4	0
4	A	80	0	112	13	0
5	A	43	0	30	2	0
6	A	15	0	16	7	0
7	A	24	0	0	3	0
All	All	4575	0	4264	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 43.

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)
1:A:512:CYS:HA	1:A:519:GLY:HA2	1.34	1.05
4:A:752:BOG:O6	3:C:1:NAG:H62	1.75	0.85
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.16	0.85
1:A:530:SER:O	1:A:534:LEU:HB2	1.76	0.85
1:A:196:LEU:HD21	1:A:392:PRO:HD3	1.61	0.83
1:A:339:GLU:HG2	1:A:562:ALA:HB2	1.60	0.82
1:A:263:PRO:HD2	1:A:285:MET:HE2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HB3	1:A:522:MET:HE1	1.62	0.81
1:A:117:LEU:HD13	1:A:366:LEU:HD21	1.63	0.80
1:A:133:ALA:HB2	4:A:752:BOG:H4	1.62	0.80
1:A:501:LEU:HD23	1:A:502:GLU:H	1.45	0.80
1:A:501:LEU:HD23	1:A:502:GLU:N	1.97	0.80
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.18	0.79
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.16	0.79
1:A:391:MET:HG3	5:A:601:COH:HAB	1.65	0.79
1:A:216:MET:HG2	3:C:2:NAG:H82	1.64	0.79
1:A:63:GLY:O	1:A:76:THR:HG21	1.83	0.78
1:A:208:GLN:NE2	1:A:228:VAL:HA	1.99	0.78
1:A:349:ALA:HB1	6:A:700:ACD:C5	2.15	0.77
1:A:73:GLU:H	1:A:76:THR:CG2	1.97	0.77
1:A:339:GLU:O	1:A:343:ILE:HG12	1.84	0.77
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.49	0.76
1:A:279:ILE:C	1:A:281:PRO:HD2	2.13	0.74
1:A:383:GLN:NE2	1:A:460:LEU:HD11	2.02	0.74
1:A:116:VAL:O	1:A:120:ARG:HB2	1.87	0.73
1:A:137:ILE:HD12	7:A:816:HOH:O	1.89	0.73
1:A:273:MET:HE2	1:A:285:MET:O	1.89	0.72
1:A:278:GLY:C	1:A:280:PRO:HD3	2.15	0.72
1:A:180:ARG:HA	1:A:180:ARG:HE	1.53	0.71
1:A:116:VAL:HG23	4:A:751:BOG:H2'2	1.72	0.71
1:A:255:GLN:OE1	1:A:257:LEU:HD21	1.90	0.71
1:A:34:ASN:HA	1:A:49:ARG:HH21	1.55	0.71
1:A:512:CYS:HA	1:A:519:GLY:CA	2.19	0.71
1:A:102:PHE:O	1:A:106:THR:HG23	1.89	0.71
1:A:130:TYR:HB3	1:A:134:HIS:O	1.91	0.70
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.28	0.69
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.72	0.69
1:A:181:PHE:CD2	1:A:487:MET:HE3	2.28	0.69
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.73	0.68
1:A:262:TYR:HB3	1:A:285:MET:CE	2.23	0.68
1:A:513:HIS:HB2	1:A:516:SER:CB	2.24	0.68
1:A:242:TYR:CD2	1:A:247:PHE:HZ	2.11	0.68
1:A:197:MET:HE2	1:A:423:VAL:HG13	1.76	0.68
1:A:308:GLU:O	1:A:311:ARG:HB3	1.94	0.68
1:A:334:LEU:HA	1:A:337:ILE:HD13	1.75	0.67
1:A:34:ASN:HA	1:A:49:ARG:NH2	2.09	0.67
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.28	0.67
1:A:521:SER:HB3	1:A:525:MET:HE3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HD11	1:A:528:PRO:HB2	1.76	0.67
1:A:163:MET:HE3	1:A:502:GLU:HG2	1.76	0.67
1:A:150:ARG:NH2	1:A:460:LEU:HD23	2.10	0.67
1:A:275:TYR:CD2	1:A:284:GLN:HG2	2.30	0.66
1:A:183:LEU:HD13	1:A:445:LEU:HD22	1.78	0.66
1:A:300:LEU:O	1:A:303:THR:HB	1.96	0.66
1:A:384:LEU:C	1:A:384:LEU:HD23	2.20	0.66
1:A:98:TRP:CE3	4:A:753:BOG:H2	2.31	0.66
1:A:202:ALA:O	1:A:206:THR:HG23	1.95	0.66
1:A:266:VAL:HA	1:A:269:ALA:O	1.96	0.65
1:A:276:PRO:O	1:A:278:GLY:N	2.28	0.65
1:A:349:ALA:HB1	6:A:700:ACD:H5	1.77	0.65
1:A:49:ARG:HH11	1:A:49:ARG:HB3	1.61	0.65
1:A:487:MET:HE1	1:A:509:LEU:HD22	1.78	0.65
1:A:216:MET:HG2	3:C:2:NAG:C8	2.25	0.65
1:A:113:MET:O	1:A:116:VAL:HG12	1.96	0.65
1:A:504:TYR:CE2	1:A:508:LEU:HD11	2.32	0.64
1:A:142:PHE:O	1:A:376:ARG:NH2	2.29	0.64
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.79	0.64
1:A:521:SER:HB3	1:A:525:MET:CE	2.27	0.64
1:A:478:PHE:CE2	1:A:491:LEU:HB3	2.33	0.64
1:A:556:PHE:CD1	1:A:560:LYS:HE3	2.33	0.64
1:A:230:LEU:C	1:A:232:HIS:H	2.04	0.64
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.32	0.64
1:A:208:GLN:NE2	1:A:230:LEU:H	1.94	0.63
1:A:195:ASN:ND2	1:A:427:SER:HA	2.13	0.63
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.63	0.62
1:A:375:ASN:OD1	1:A:533:GLY:HA3	2.00	0.62
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.33	0.62
1:A:151:ILE:HD11	1:A:529:PHE:HE2	1.65	0.62
1:A:327:GLN:C	1:A:329:PHE:H	2.08	0.61
1:A:442:HIS:HD2	1:A:443:HIS:H	1.48	0.61
1:A:151:ILE:HD11	1:A:529:PHE:CE2	2.35	0.61
1:A:107:PHE:C	1:A:109:ARG:H	2.07	0.61
1:A:513:HIS:NE2	1:A:520:GLU:HA	2.15	0.61
1:A:74:ILE:HG23	1:A:75:TRP:H	1.66	0.61
1:A:114:ARG:HG3	1:A:365:LEU:O	2.01	0.61
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.81	0.61
1:A:193:GLY:O	1:A:582:VAL:HG12	2.01	0.60
1:A:230:LEU:HD21	1:A:336:LEU:HB3	1.82	0.60
1:A:258:ASN:HD21	1:A:415:VAL:HG12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:HIS:CD2	1:A:232:HIS:CD2	2.89	0.60
1:A:289:GLN:HB3	1:A:292:PHE:CD2	2.37	0.60
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.84	0.60
1:A:245:ARG:HB2	1:A:247:PHE:CE1	2.37	0.60
1:A:252:LEU:HD11	1:A:329:PHE:HE1	1.67	0.59
1:A:323:TRP:CD2	1:A:327:GLN:HG2	2.38	0.59
1:A:568:VAL:HG12	1:A:569:CYS:N	2.16	0.59
1:A:263:PRO:HD2	1:A:285:MET:CE	2.32	0.59
1:A:96:GLY:O	1:A:97:ARG:C	2.45	0.59
1:A:298:LEU:N	1:A:298:LEU:HD12	2.17	0.59
1:A:107:PHE:C	1:A:109:ARG:N	2.60	0.59
1:A:130:TYR:HB2	1:A:150:ARG:HG3	1.84	0.58
1:A:181:PHE:HD2	1:A:487:MET:HE3	1.67	0.58
1:A:171:LEU:HB3	1:A:456:ARG:NH2	2.18	0.58
1:A:43:HIS:O	1:A:44:GLN:HB2	2.02	0.58
1:A:262:TYR:HB3	1:A:285:MET:HE1	1.84	0.58
1:A:43:HIS:HA	7:A:810:HOH:O	2.04	0.58
1:A:145:VAL:HG12	1:A:226:HIS:HE2	1.69	0.58
1:A:484:GLU:OE2	1:A:487:MET:N	2.37	0.58
1:A:150:ARG:HH22	1:A:460:LEU:HD23	1.67	0.57
1:A:88:PHE:O	1:A:91:PHE:HB3	2.04	0.57
1:A:91:PHE:CE2	4:A:750:BOG:H3'2	2.40	0.57
1:A:561:THR:HG22	1:A:561:THR:O	2.04	0.57
1:A:373:TYR:CZ	1:A:541:SER:HA	2.40	0.57
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.86	0.57
1:A:333:ARG:HG2	1:A:337:ILE:HD11	1.87	0.57
1:A:117:LEU:CD1	1:A:366:LEU:HD21	2.34	0.57
1:A:178:SER:OG	1:A:449:VAL:HG22	2.05	0.57
1:A:120:ARG:HD3	6:A:700:ACD:O2	2.04	0.56
1:A:209:PHE:HB3	1:A:227:GLY:H	1.70	0.56
1:A:337:ILE:HD12	1:A:337:ILE:N	2.19	0.56
1:A:408:LEU:C	1:A:410:ASN:H	2.13	0.56
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.87	0.56
1:A:274:HIS:HD2	1:A:290:GLU:HB3	1.70	0.56
1:A:380:GLU:OE1	1:A:380:GLU:N	2.30	0.56
1:A:513:HIS:CE1	1:A:520:GLU:HA	2.40	0.56
1:A:100:TRP:O	1:A:104:ASN:HB2	2.05	0.56
1:A:305:TRP:HE3	1:A:336:LEU:HD13	1.70	0.56
1:A:150:ARG:NH2	1:A:379:MET:SD	2.78	0.56
1:A:299:MET:HG3	1:A:414:LEU:HD23	1.86	0.56
1:A:254:TYR:CD1	1:A:261:VAL:HG13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HB3	1:A:462:PRO:HD2	1.85	0.56
1:A:501:LEU:HD22	1:A:502:GLU:O	2.06	0.56
1:A:112:LEU:HD22	4:A:751:BOG:H6'1	1.88	0.56
1:A:305:TRP:CE3	1:A:336:LEU:HD13	2.40	0.55
1:A:395:PHE:HE1	1:A:404:TYR:CE2	2.24	0.55
1:A:116:VAL:HA	4:A:751:BOG:H2'2	1.86	0.55
1:A:201:PHE:CD2	1:A:201:PHE:C	2.84	0.55
1:A:375:ASN:ND2	1:A:376:ARG:H	2.04	0.55
1:A:414:LEU:HD12	1:A:414:LEU:O	2.05	0.55
1:A:73:GLU:N	1:A:76:THR:CG2	2.67	0.55
1:A:116:VAL:HG23	4:A:751:BOG:C2'	2.36	0.55
4:A:752:BOG:O6	3:C:1:NAG:C6	2.52	0.55
1:A:338:GLY:HA3	1:A:559:VAL:HG13	1.89	0.55
1:A:344:VAL:O	1:A:348:TYR:HB3	2.07	0.55
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.71	0.55
1:A:204:HIS:CD2	1:A:232:HIS:HD2	2.25	0.54
1:A:564:LEU:HD22	1:A:578:VAL:CG2	2.37	0.54
1:A:74:ILE:HG23	1:A:75:TRP:N	2.20	0.54
1:A:388:HIS:N	1:A:389:PRO:HD2	2.22	0.54
1:A:444:ILE:O	1:A:447:VAL:HG23	2.07	0.54
1:A:390:LEU:HD21	1:A:434:ILE:HD11	1.89	0.54
1:A:319:GLU:HB3	1:A:320:HIS:ND1	2.23	0.54
1:A:196:LEU:HD11	1:A:429:GLN:NE2	2.23	0.54
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.43	0.54
1:A:408:LEU:O	1:A:410:ASN:N	2.41	0.54
1:A:501:LEU:CD2	1:A:502:GLU:N	2.67	0.54
1:A:150:ARG:NH1	1:A:154:SER:HA	2.22	0.54
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.22	0.53
1:A:387:PHE:HB3	1:A:390:LEU:HG	1.90	0.53
1:A:163:MET:HG2	1:A:171:LEU:HD21	1.89	0.53
1:A:523:ILE:CG2	6:A:700:ACD:H8	2.39	0.53
1:A:395:PHE:CD1	1:A:395:PHE:N	2.77	0.53
1:A:442:HIS:NE2	1:A:443:HIS:CE1	2.76	0.53
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.24	0.53
1:A:204:HIS:NE2	1:A:232:HIS:CD2	2.77	0.53
1:A:299:MET:HG3	1:A:414:LEU:CD2	2.39	0.53
1:A:178:SER:CB	1:A:449:VAL:HG22	2.39	0.53
1:A:251:LYS:HB3	1:A:310:ASN:OD1	2.08	0.53
1:A:282:GLN:C	1:A:284:GLN:H	2.17	0.53
1:A:294:LEU:O	1:A:295:LEU:HG	2.09	0.52
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:O	1:A:459:ARG:HB2	2.09	0.52
1:A:168:LYS:C	1:A:170:GLN:H	2.17	0.52
1:A:280:PRO:N	1:A:281:PRO:HD2	2.25	0.52
1:A:487:MET:HE1	1:A:509:LEU:CD2	2.38	0.52
1:A:514:PRO:O	1:A:515:ASN:HB2	2.10	0.52
1:A:183:LEU:CD1	1:A:445:LEU:HD22	2.40	0.52
1:A:384:LEU:HD23	1:A:384:LEU:O	2.10	0.52
1:A:197:MET:HB2	1:A:427:SER:HA	1.91	0.52
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.44	0.52
1:A:148:TYR:CE1	1:A:221:THR:HB	2.45	0.52
1:A:201:PHE:C	1:A:201:PHE:HD2	2.18	0.52
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.45	0.52
1:A:433:ARG:HD3	1:A:435:GLY:O	2.10	0.51
1:A:442:HIS:CD2	1:A:443:HIS:N	2.79	0.51
1:A:230:LEU:CD2	1:A:336:LEU:HB3	2.40	0.51
1:A:295:LEU:HD11	5:A:601:COH:HBB1	1.91	0.51
1:A:297:GLY:O	1:A:300:LEU:HB3	2.11	0.51
1:A:564:LEU:HD23	1:A:564:LEU:O	2.11	0.51
1:A:566:LYS:O	1:A:570:LEU:HB2	2.10	0.51
1:A:403:SER:H	1:A:406:GLN:CG	2.24	0.51
1:A:442:HIS:HE2	1:A:443:HIS:CE1	2.28	0.51
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.26	0.51
1:A:126:SER:HA	1:A:127:PRO:C	2.36	0.51
1:A:150:ARG:NH1	1:A:154:SER:OG	2.43	0.51
1:A:292:PHE:CD1	1:A:298:LEU:HB3	2.46	0.51
1:A:296:PRO:HD2	1:A:407:PHE:CZ	2.46	0.51
1:A:329:PHE:HD2	1:A:330:GLN:NE2	2.09	0.51
1:A:582:VAL:HG22	1:A:583:PRO:O	2.11	0.51
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.50	0.51
1:A:204:HIS:HE2	1:A:232:HIS:CD2	2.29	0.51
1:A:453:LYS:O	1:A:457:VAL:HG23	2.11	0.50
1:A:200:PHE:CE1	1:A:391:MET:HE1	2.46	0.50
1:A:298:LEU:N	1:A:298:LEU:CD1	2.74	0.50
1:A:184:ARG:HH12	1:A:392:PRO:C	2.19	0.50
1:A:379:MET:O	1:A:382:ASN:HB3	2.12	0.50
1:A:155:VAL:O	1:A:156:PRO:C	2.54	0.50
1:A:183:LEU:HD13	1:A:445:LEU:CD2	2.40	0.50
1:A:197:MET:HG3	1:A:427:SER:OG	2.12	0.50
1:A:245:ARG:NH2	1:A:325:ASP:OD2	2.44	0.50
1:A:442:HIS:HD2	1:A:443:HIS:N	2.09	0.50
1:A:251:LYS:HB3	1:A:310:ASN:CG	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:GLN:C	1:A:329:PHE:N	2.69	0.50
1:A:112:LEU:O	1:A:115:LEU:N	2.44	0.50
1:A:274:HIS:CD2	1:A:290:GLU:HB3	2.47	0.50
1:A:493:GLU:O	1:A:494:LEU:HG	2.12	0.49
1:A:380:GLU:HG2	1:A:466:TYR:CZ	2.47	0.49
1:A:422:LEU:HD13	1:A:426:PHE:CE2	2.46	0.49
1:A:550:PHE:CE2	1:A:559:VAL:HG21	2.46	0.49
1:A:298:LEU:CD1	1:A:298:LEU:H	2.26	0.49
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.47	0.49
1:A:109:ARG:NH2	1:A:360:LYS:HB2	2.28	0.49
1:A:383:GLN:OE1	1:A:455:SER:HB2	2.13	0.49
1:A:123:LEU:O	1:A:469:ARG:NH2	2.46	0.49
1:A:131:ASN:OD1	1:A:134:HIS:N	2.45	0.49
1:A:98:TRP:HB2	4:A:753:BOG:O2	2.12	0.49
1:A:166:LYS:HE3	1:A:497:ASP:OD1	2.12	0.49
1:A:230:LEU:HA	1:A:232:HIS:ND1	2.27	0.49
1:A:107:PHE:H	1:A:107:PHE:HD2	1.61	0.49
1:A:334:LEU:CA	1:A:337:ILE:HD13	2.41	0.49
1:A:549:THR:HG22	1:A:549:THR:O	2.13	0.49
1:A:338:GLY:CA	1:A:559:VAL:HG13	2.41	0.49
1:A:403:SER:H	1:A:406:GLN:CD	2.21	0.49
1:A:537:ASN:OD1	1:A:539:ILE:HG12	2.13	0.48
1:A:204:HIS:ND1	1:A:301:TYR:HB3	2.29	0.48
1:A:98:TRP:HE3	4:A:753:BOG:H2	1.73	0.48
1:A:204:HIS:NE2	1:A:232:HIS:HD2	2.11	0.48
1:A:179:ARG:HA	1:A:183:LEU:HB2	1.96	0.48
1:A:200:PHE:CD1	1:A:391:MET:HE1	2.48	0.48
1:A:541:SER:HB2	1:A:542:PRO:HD2	1.96	0.48
1:A:511:LYS:O	1:A:511:LYS:HG3	2.14	0.48
1:A:423:VAL:C	1:A:425:ALA:N	2.72	0.48
1:A:535:LEU:HD13	1:A:540:CYS:SG	2.54	0.48
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.49	0.47
1:A:383:GLN:NE2	1:A:460:LEU:CD1	2.74	0.47
1:A:384:LEU:C	1:A:384:LEU:CD2	2.87	0.47
1:A:107:PHE:O	1:A:109:ARG:N	2.48	0.47
1:A:47:CYS:O	1:A:48:VAL:HG13	2.13	0.47
1:A:242:TYR:CD2	1:A:247:PHE:CZ	2.99	0.47
1:A:152:LEU:HD21	1:A:469:ARG:HG3	1.96	0.47
1:A:171:LEU:HB3	1:A:456:ARG:HH21	1.79	0.47
1:A:149:THR:O	1:A:378:ALA:HA	2.14	0.47
1:A:237:ASN:ND2	1:A:240:ARG:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HG	1:A:246:LEU:O	2.14	0.47
1:A:333:ARG:O	1:A:336:LEU:N	2.38	0.47
1:A:419:VAL:O	1:A:420:GLU:C	2.56	0.47
1:A:543:GLU:O	1:A:546:LYS:HE3	2.15	0.47
1:A:568:VAL:O	1:A:572:THR:HG23	2.15	0.47
1:A:152:LEU:HD12	1:A:466:TYR:CZ	2.50	0.47
1:A:180:ARG:HA	1:A:180:ARG:NE	2.26	0.47
1:A:131:ASN:HB2	1:A:147:TYR:CD1	2.49	0.47
1:A:75:TRP:CE3	1:A:78:LEU:HD12	2.50	0.47
1:A:230:LEU:C	1:A:232:HIS:N	2.72	0.47
1:A:538:PRO:HB2	1:A:544:TYR:CE1	2.50	0.46
1:A:329:PHE:HD2	1:A:330:GLN:HE21	1.63	0.46
1:A:523:ILE:HG22	6:A:700:ACD:H8	1.96	0.46
1:A:291:VAL:HG22	1:A:291:VAL:O	2.16	0.46
1:A:149:THR:HG22	1:A:377:ILE:O	2.16	0.46
1:A:261:VAL:C	1:A:262:TYR:CD1	2.93	0.46
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.80	0.46
1:A:306:LEU:HD23	1:A:306:LEU:C	2.41	0.46
1:A:482:THR:HG22	1:A:509:LEU:O	2.16	0.46
6:A:700:ACD:H41	6:A:700:ACD:H71	1.77	0.46
1:A:504:TYR:N	1:A:505:PRO:CD	2.79	0.46
1:A:408:LEU:C	1:A:410:ASN:N	2.71	0.46
1:A:198:PHE:HA	1:A:580:PHE:CD1	2.51	0.45
1:A:409:PHE:C	1:A:410:ASN:O	2.59	0.45
1:A:424:ASP:O	1:A:428:ARG:HD2	2.15	0.45
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.51	0.45
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.51	0.45
1:A:527:ALA:HB3	1:A:528:PRO:CD	2.46	0.45
1:A:415:VAL:HG12	1:A:415:VAL:O	2.16	0.45
2:B:1:NAG:O6	2:B:2:NDG:H8C1	2.17	0.45
1:A:308:GLU:O	1:A:309:HIS:C	2.57	0.45
1:A:338:GLY:O	1:A:339:GLU:C	2.58	0.45
1:A:417:TYR:HD2	7:A:821:HOH:O	2.00	0.45
1:A:564:LEU:HD23	1:A:564:LEU:C	2.42	0.45
1:A:73:GLU:O	1:A:74:ILE:C	2.59	0.45
1:A:337:ILE:HD12	1:A:337:ILE:H	1.81	0.45
1:A:532:LYS:HD2	1:A:532:LYS:O	2.17	0.45
1:A:163:MET:CE	1:A:502:GLU:HG2	2.43	0.44
1:A:203:GLN:O	1:A:204:HIS:C	2.60	0.44
1:A:255:GLN:HE21	1:A:264:PRO:HA	1.81	0.44
1:A:582:VAL:HG23	1:A:583:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HB	1:A:58:ASP:HB3	1.99	0.44
1:A:150:ARG:NH2	1:A:460:LEU:CD2	2.79	0.44
1:A:197:MET:SD	1:A:301:TYR:OH	2.73	0.44
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.53	0.44
1:A:120:ARG:HH22	1:A:524:GLU:CD	2.26	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CE1	2.53	0.44
1:A:204:HIS:ND1	1:A:301:TYR:CB	2.80	0.44
1:A:574:THR:O	1:A:576:PRO:HD3	2.18	0.44
1:A:409:PHE:O	1:A:410:ASN:C	2.61	0.44
1:A:225:GLY:O	1:A:226:HIS:O	2.35	0.44
1:A:319:GLU:HB3	1:A:320:HIS:CE1	2.52	0.44
1:A:544:TYR:O	1:A:546:LYS:N	2.49	0.44
1:A:107:PHE:CD2	1:A:107:PHE:N	2.86	0.43
1:A:115:LEU:O	1:A:119:VAL:HG23	2.17	0.43
1:A:255:GLN:NE2	1:A:265:SER:N	2.66	0.43
1:A:462:PRO:O	1:A:465:GLU:HB2	2.18	0.43
1:A:179:ARG:O	1:A:183:LEU:HB3	2.19	0.43
1:A:402:TYR:CD2	1:A:402:TYR:N	2.86	0.43
1:A:224:LEU:C	1:A:226:HIS:H	2.27	0.43
1:A:246:LEU:O	1:A:248:LYS:N	2.52	0.43
1:A:329:PHE:CD2	1:A:330:GLN:NE2	2.86	0.43
1:A:363:PRO:HG2	1:A:545:TRP:CE2	2.54	0.43
1:A:308:GLU:O	1:A:311:ARG:N	2.52	0.43
1:A:108:ILE:O	1:A:112:LEU:HG	2.18	0.43
1:A:136:TYR:CD1	1:A:136:TYR:C	2.97	0.43
1:A:162:PRO:HG3	1:A:171:LEU:HG	2.01	0.43
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.48	0.43
1:A:279:ILE:C	1:A:281:PRO:CD	2.89	0.43
1:A:244:LEU:HD12	1:A:244:LEU:O	2.19	0.43
1:A:454:GLU:O	1:A:457:VAL:HB	2.19	0.43
1:A:201:PHE:CE2	1:A:205:PHE:HB2	2.53	0.43
1:A:305:TRP:O	1:A:308:GLU:HB3	2.19	0.43
1:A:183:LEU:HB2	1:A:445:LEU:CD2	2.49	0.42
1:A:60:THR:C	1:A:62:THR:H	2.27	0.42
1:A:208:GLN:HE21	1:A:229:ASP:H	1.66	0.42
1:A:343:ILE:HD12	1:A:563:THR:C	2.43	0.42
1:A:144:ASN:OD1	1:A:146:SER:CB	2.68	0.42
1:A:448:ALA:O	1:A:452:ILE:HG22	2.19	0.42
1:A:245:ARG:O	1:A:247:PHE:HD1	2.02	0.42
1:A:246:LEU:O	1:A:246:LEU:CG	2.66	0.42
1:A:462:PRO:O	1:A:463:PHE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:HB3	1:A:487:MET:CE	2.50	0.42
1:A:363:PRO:HB3	1:A:540:CYS:O	2.18	0.42
1:A:483:GLY:H	1:A:511:LYS:HB3	1.84	0.42
1:A:375:ASN:OD1	1:A:533:GLY:CA	2.67	0.42
1:A:176:PHE:O	1:A:177:LEU:C	2.63	0.42
1:A:331:THR:HG23	1:A:550:PHE:HA	2.02	0.42
1:A:564:LEU:HD22	1:A:578:VAL:HG21	2.01	0.42
1:A:210:PHE:CZ	1:A:382:ASN:HA	2.55	0.42
1:A:275:TYR:CG	1:A:284:GLN:HG2	2.54	0.42
1:A:358:GLN:O	1:A:359:LEU:C	2.62	0.42
1:A:567:LEU:HA	1:A:567:LEU:HD12	1.77	0.42
1:A:423:VAL:C	1:A:425:ALA:H	2.27	0.42
1:A:440:ILE:HD13	1:A:448:ALA:HB2	2.02	0.42
1:A:507:LEU:HD22	1:A:522:MET:CE	2.49	0.42
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.55	0.42
1:A:495:TYR:OH	1:A:502:GLU:HG3	2.20	0.41
1:A:582:VAL:CG2	1:A:583:PRO:N	2.81	0.41
1:A:291:VAL:O	1:A:293:GLY:N	2.53	0.41
1:A:439:ASN:HD22	1:A:439:ASN:HA	1.54	0.41
6:A:700:ACD:H102	6:A:700:ACD:H72	1.80	0.41
1:A:75:TRP:O	1:A:78:LEU:N	2.53	0.41
1:A:211:LYS:HE3	1:A:223:ALA:HB2	2.02	0.41
1:A:255:GLN:HE21	1:A:265:SER:N	2.18	0.41
1:A:410:ASN:OD1	1:A:411:THR:N	2.53	0.41
1:A:59:CYS:O	1:A:62:THR:CB	2.68	0.41
1:A:414:LEU:HD12	1:A:414:LEU:C	2.45	0.41
1:A:487:MET:CE	1:A:509:LEU:HD22	2.48	0.41
1:A:60:THR:C	1:A:62:THR:N	2.77	0.41
1:A:299:MET:O	1:A:300:LEU:C	2.64	0.41
1:A:195:ASN:O	1:A:198:PHE:HB3	2.21	0.41
1:A:218:PRO:HB3	1:A:454:GLU:HG3	2.01	0.41
1:A:34:ASN:C	1:A:34:ASN:OD1	2.63	0.41
1:A:73:GLU:H	1:A:76:THR:HG21	1.81	0.41
1:A:115:LEU:HD23	4:A:751:BOG:H5'2	2.02	0.41
1:A:116:VAL:CG1	1:A:117:LEU:N	2.84	0.41
1:A:275:TYR:CE2	1:A:284:GLN:HG2	2.55	0.41
1:A:518:PHE:HE2	1:A:523:ILE:HG12	1.85	0.41
1:A:564:LEU:C	1:A:564:LEU:CD2	2.94	0.41
1:A:133:ALA:HB1	4:A:752:BOG:H2	2.02	0.41
1:A:150:ARG:NH1	1:A:154:SER:CA	2.83	0.41
1:A:280:PRO:O	1:A:284:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA3	1:A:559:VAL:CG1	2.50	0.41
1:A:306:LEU:O	1:A:307:ARG:C	2.65	0.40
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.93	0.40
1:A:200:PHE:O	1:A:201:PHE:C	2.63	0.40
1:A:253:LYS:O	1:A:254:TYR:HB3	2.21	0.40
1:A:531:LEU:O	1:A:532:LYS:C	2.64	0.40
1:A:383:GLN:HE22	1:A:460:LEU:CD1	2.34	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	551/600 (92%)	428 (78%)	91 (16%)	32 (6%)	1 8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	247	PHE
1	A	277	ARG
1	A	281	PRO
1	A	409	PHE
1	A	545	TRP
1	A	169	LYS
1	A	292	PHE
1	A	420	GLU
1	A	551	GLY
1	A	117	LEU
1	A	160	PRO
1	A	173	ASP
1	A	317	LYS

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Mol	Chain	Res	Type
1	A	401	ASP
1	A	486	GLU
1	A	569	CYS
1	A	93	LEU
1	A	223	ALA
1	A	290	GLU
1	A	382	ASN
1	A	392	PRO
1	A	419	VAL
1	A	445	LEU
1	A	494	LEU
1	A	204	HIS
1	A	328	LEU
1	A	350	GLN
1	A	400	GLN
1	A	280	PRO
1	A	270	PRO
1	A	74	ILE

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	435/529 (82%)	386 (89%)	49 (11%)	5 23

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	46	ILE
1	A	48	VAL
1	A	49	ARG
1	A	106	THR
1	A	107	PHE
1	A	110	ASP
1	A	114	ARG

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Mol	Chain	Res	Type
1	A	116	VAL
1	A	120	ARG
1	A	136	TYR
1	A	140	GLU
1	A	145	VAL
1	A	148	TYR
1	A	177	LEU
1	A	180	ARG
1	A	197	MET
1	A	201	PHE
1	A	228	VAL
1	A	244	LEU
1	A	257	LEU
1	A	272	LEU
1	A	280	PRO
1	A	284	GLN
1	A	307	ARG
1	A	312	VAL
1	A	322	THR
1	A	336	LEU
1	A	342	LYS
1	A	366	LEU
1	A	376	ARG
1	A	384	LEU
1	A	395	PHE
1	A	422	LEU
1	A	439	ASN
1	A	452	ILE
1	A	469	ARG
1	A	484	GLU
1	A	501	LEU
1	A	518	PHE
1	A	523	ILE
1	A	534	LEU
1	A	535	LEU
1	A	554	VAL
1	A	556	PHE
1	A	570	LEU
1	A	574	THR
1	A	578	VAL
1	A	582	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	56	GLN
1	A	90	HIS
1	A	203	GLN
1	A	208	GLN
1	A	232	HIS
1	A	255	GLN
1	A	258	ASN
1	A	274	HIS
1	A	330	GLN
1	A	358	GLN
1	A	375	ASN
1	A	382	ASN
1	A	383	GLN
1	A	406	GLN
1	A	439	ASN
1	A	443	HIS
1	A	557	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](#)

8 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	2,1	14,14,15	0.76	0	17,19,21	1.19	3 (17%)
2	NDG	B	2	2	14,14,15	0.93	1 (7%)	17,19,21	0.83	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	0.79	1 (5%)
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	0.87	0
3	BMA	C	3	3	11,11,12	0.52	0	15,15,17	0.43	0
3	BMA	C	4	3	11,11,12	0.72	0	15,15,17	0.88	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.67	0	17,19,21	0.69	0
2	NDG	D	2	2	14,14,15	0.79	1 (7%)	17,19,21	0.98	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	2,1	-	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	-	0/2/19/22	0/1/1/1
3	BMA	C	4	3	-	2/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	5/6/23/26	0/1/1/1
2	NDG	D	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NDG	C1-C2	2.96	1.56	1.52
2	D	2	NDG	C1-C2	2.10	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	BMA	C1-O5-C5	3.01	116.22	112.19
2	B	1	NAG	C2-N2-C7	-2.97	118.92	122.90
3	C	1	NAG	C2-N2-C7	-2.46	119.61	122.90
2	B	1	NAG	C4-C3-C2	-2.17	107.84	111.02
2	D	2	NDG	C2-N2-C7	-2.11	120.07	122.90
2	B	2	NDG	C2-N2-C7	-2.08	120.11	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

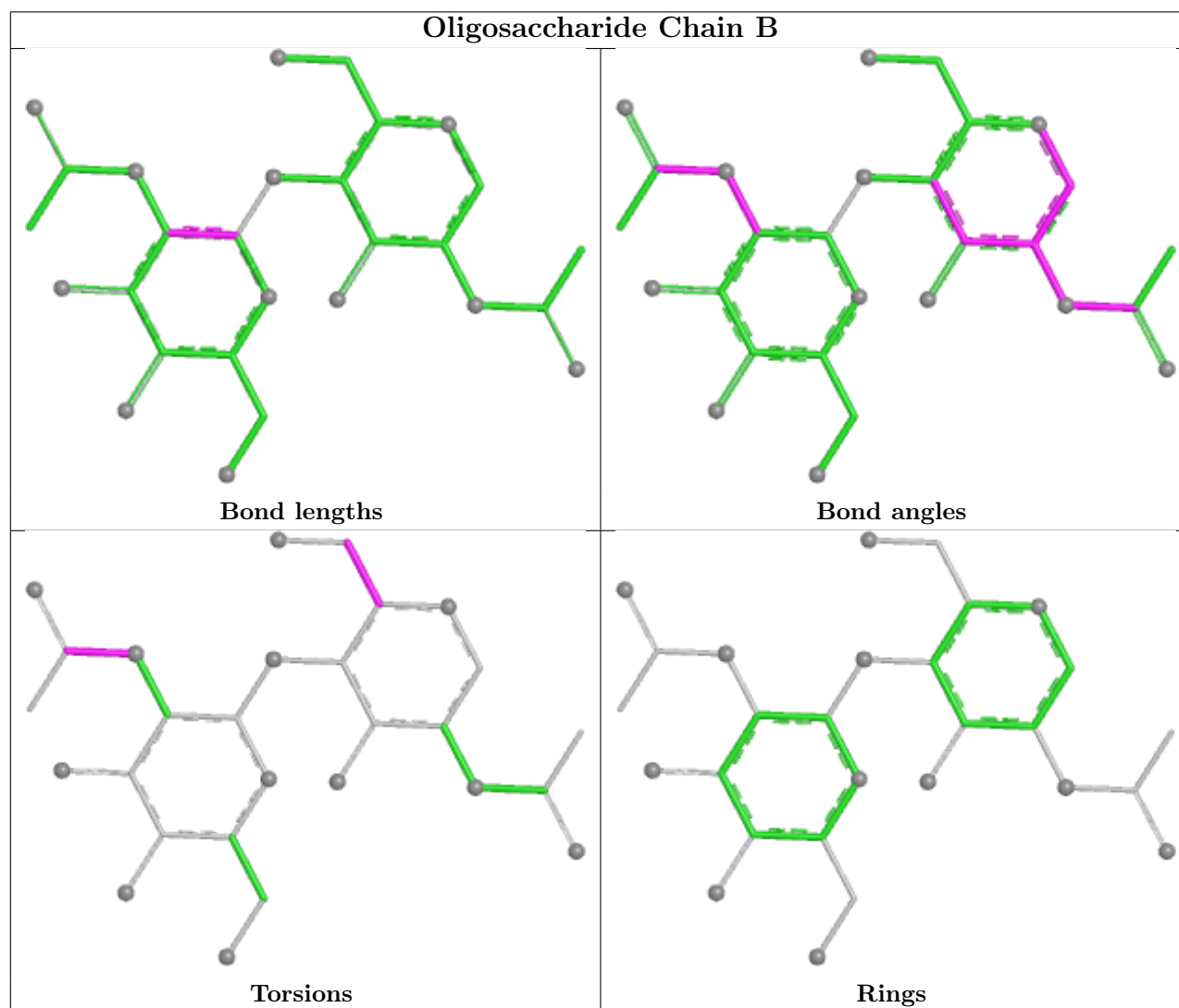
All (1) ring outliers are listed below:

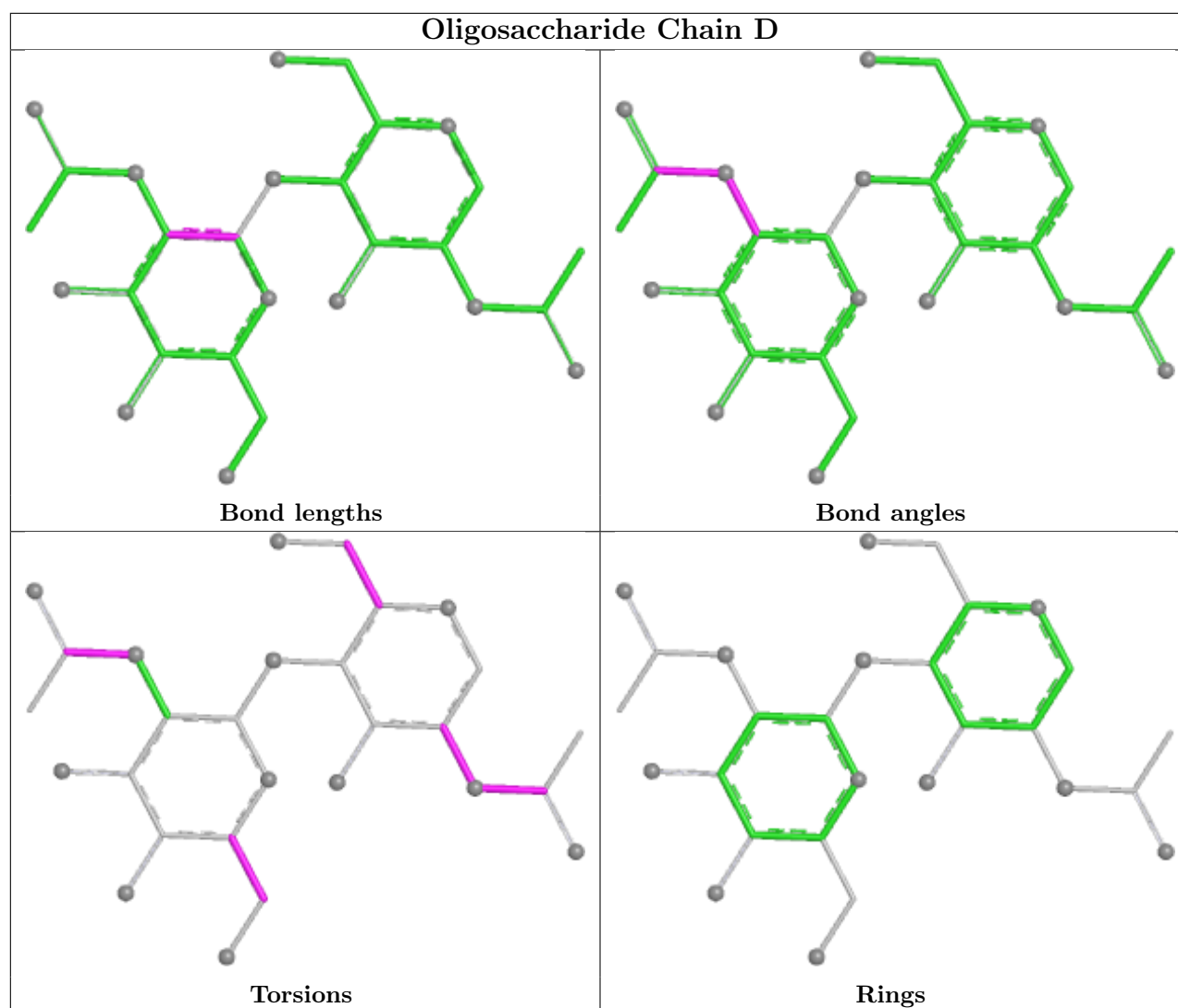
Mol	Chain	Res	Type	Atoms
3	C	4	BMA	C1-C2-C3-C4-C5-O5

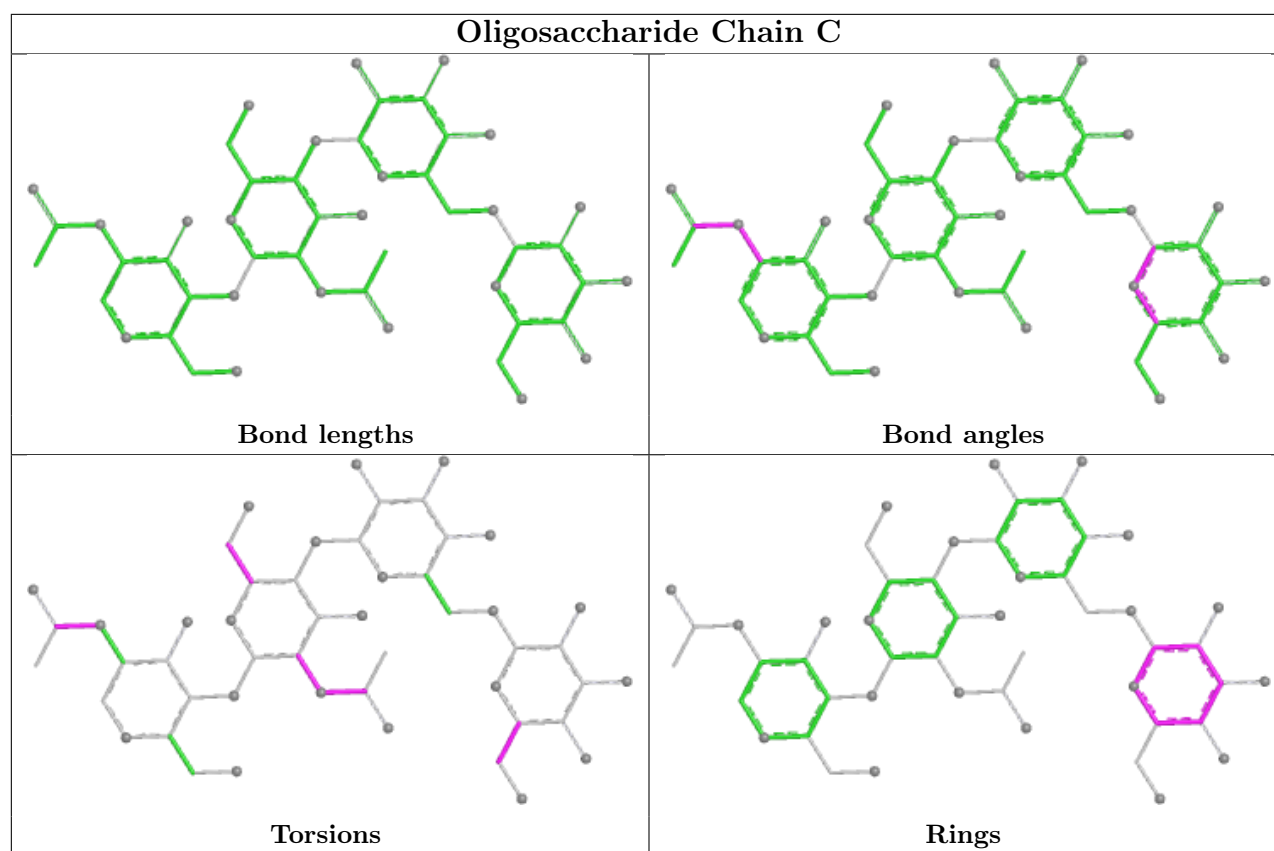
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NDG	1	0
3	C	2	NAG	2	0
3	C	1	NAG	2	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	$\# Z > 2$
4	BOG	A	751	-	20,20,20	0.42	0	25,25,25	0.88	2 (8%)
4	BOG	A	753	-	20,20,20	0.50	0	25,25,25	0.81	1 (4%)
4	BOG	A	750	-	20,20,20	0.39	0	25,25,25	0.67	1 (4%)
5	COH	A	601	1	50,50,50	1.98	12 (24%)	66,82,82	1.56	14 (21%)
4	BOG	A	752	-	20,20,20	0.49	0	25,25,25	0.57	0
6	ACD	A	700	-	14,14,21	0.84	0	14,14,21	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	A	751	-	-	3/11/31/31	0/1/1/1
4	BOG	A	753	-	-	6/11/31/31	0/1/1/1
4	BOG	A	750	-	-	3/11/31/31	0/1/1/1
5	COH	A	601	1	1/1/3/9	8/14/54/54	-
4	BOG	A	752	-	-	3/11/31/31	0/1/1/1
6	ACD	A	700	-	-	5/12/12/19	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COH	C1D-C2D	5.27	1.55	1.43
5	A	601	COH	C1A-C2A	5.03	1.53	1.45
5	A	601	COH	C4A-C3A	4.69	1.54	1.44
5	A	601	COH	CAA-C2A	3.74	1.61	1.51
5	A	601	COH	C4D-ND	3.45	1.44	1.38
5	A	601	COH	C2A-C3A	3.03	1.43	1.36
5	A	601	COH	CMC-C2C	2.95	1.56	1.50
5	A	601	COH	CBC-CAC	2.81	1.43	1.30
5	A	601	COH	C4C-NC	-2.65	1.34	1.39
5	A	601	COH	CHB-C4A	-2.16	1.34	1.39
5	A	601	COH	CO-NC	2.14	2.04	1.96
5	A	601	COH	C1D-ND	-2.08	1.35	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	COH	C2B-C1B-NB	4.44	114.33	110.88
5	A	601	COH	CMD-C2D-C3D	3.65	133.37	125.62
5	A	601	COH	C4A-C3A-C2A	-3.44	103.37	106.98
5	A	601	COH	C3A-C4A-NA	3.40	114.50	110.96
5	A	601	COH	CAA-C2A-C1A	3.05	130.02	124.70
5	A	601	COH	CHC-C4B-NB	-2.68	121.67	124.85
5	A	601	COH	C4B-NB-C1B	-2.65	101.21	105.11
4	A	750	BOG	C1'-O1-C1	2.64	118.19	113.68
5	A	601	COH	C1D-C2D-C3D	-2.51	103.95	106.82
5	A	601	COH	C2D-C1D-ND	2.49	112.12	109.69
5	A	601	COH	C4C-C3C-C2C	-2.43	105.05	107.28
4	A	751	BOG	C1'-O1-C1	2.37	117.73	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	COH	CHB-C1B-NB	-2.34	122.08	124.85
5	A	601	COH	CHB-C4A-C3A	-2.17	121.60	125.03
5	A	601	COH	C3B-C2B-C1B	-2.14	105.02	107.05
4	A	751	BOG	C3-C4-C5	2.07	113.98	110.23
5	A	601	COH	CAA-C2A-C3A	-2.06	124.01	127.87
4	A	753	BOG	C3-C4-C5	-2.03	106.56	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	COH	NB

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	750	BOG	C2'-C1'-O1-C1
4	A	751	BOG	C2'-C1'-O1-C1
4	A	753	BOG	C2-C1-O1-C1'
4	A	753	BOG	O5-C1-O1-C1'
4	A	752	BOG	O5-C5-C6-O6
4	A	753	BOG	O5-C5-C6-O6
4	A	752	BOG	C4-C5-C6-O6
4	A	753	BOG	C4-C5-C6-O6
4	A	750	BOG	O5-C5-C6-O6
4	A	751	BOG	O5-C1-O1-C1'
4	A	752	BOG	C2'-C1'-O1-C1
4	A	753	BOG	C4'-C5'-C6'-C7'
4	A	751	BOG	C1'-C2'-C3'-C4'
4	A	753	BOG	C2'-C1'-O1-C1
6	A	700	ACD	C9-C10-C11-C12
5	A	601	COH	C2B-C3B-CAB-CBB
5	A	601	COH	C2C-C3C-CAC-CBC
6	A	700	ACD	C1-C2-C3-C4
5	A	601	COH	C4B-C3B-CAB-CBB
4	A	750	BOG	C4-C5-C6-O6
6	A	700	ACD	C11-C10-C9-C8
6	A	700	ACD	O1-C1-C2-C3
6	A	700	ACD	O2-C1-C2-C3
5	A	601	COH	CAA-CBA-CGA-O2A
5	A	601	COH	C4C-C3C-CAC-CBC
5	A	601	COH	CAA-CBA-CGA-O1A
5	A	601	COH	CAD-CBD-CGD-O2D

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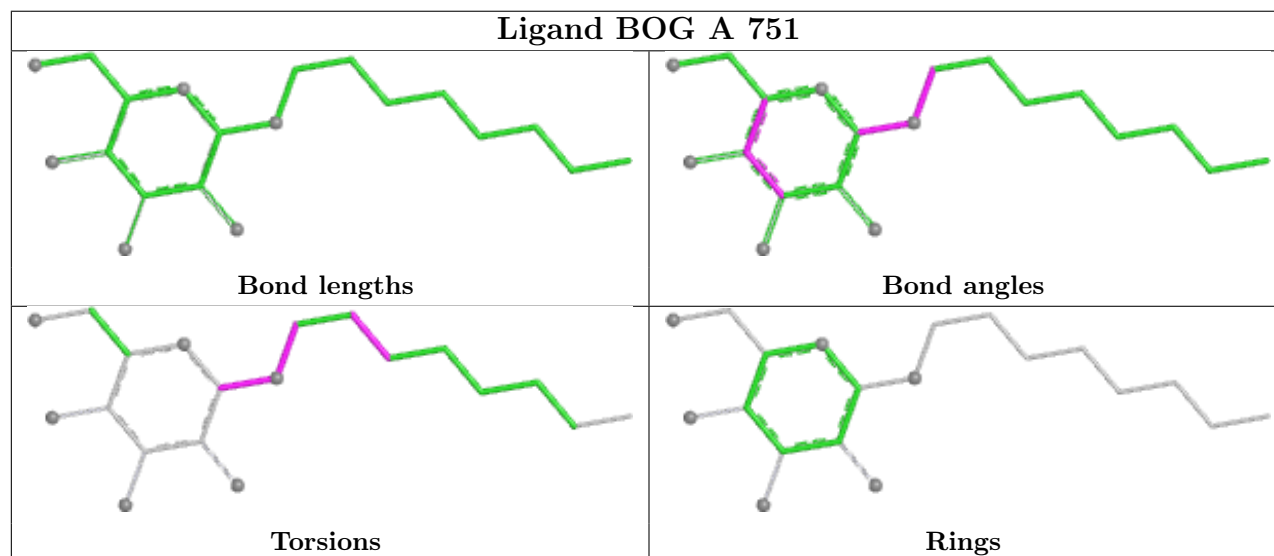
Mol	Chain	Res	Type	Atoms
5	A	601	COH	CAD-CBD-CGD-O1D

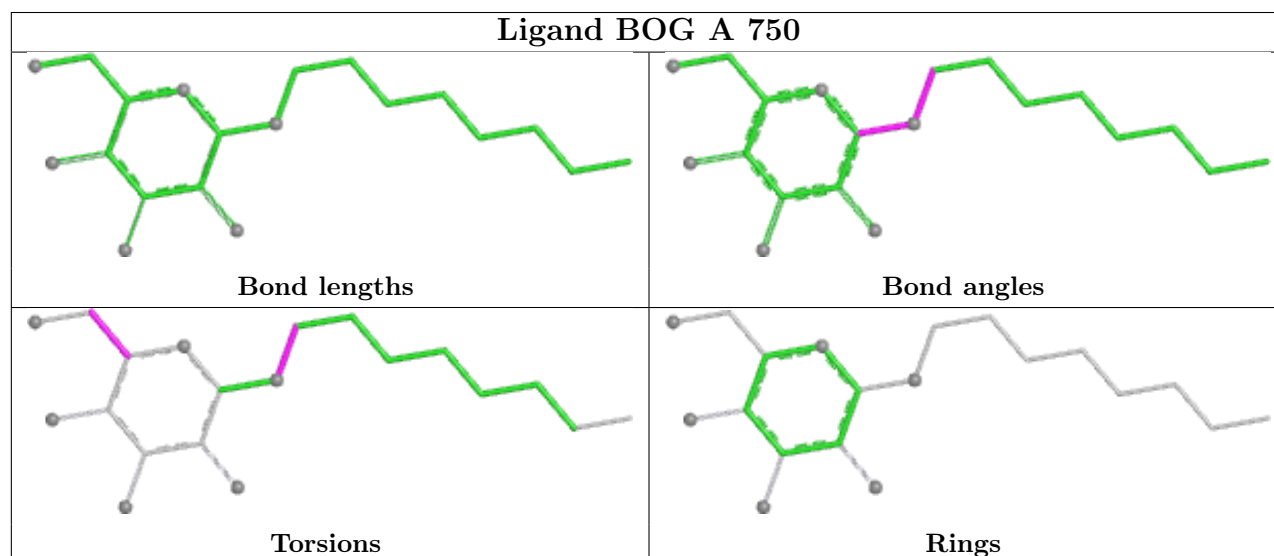
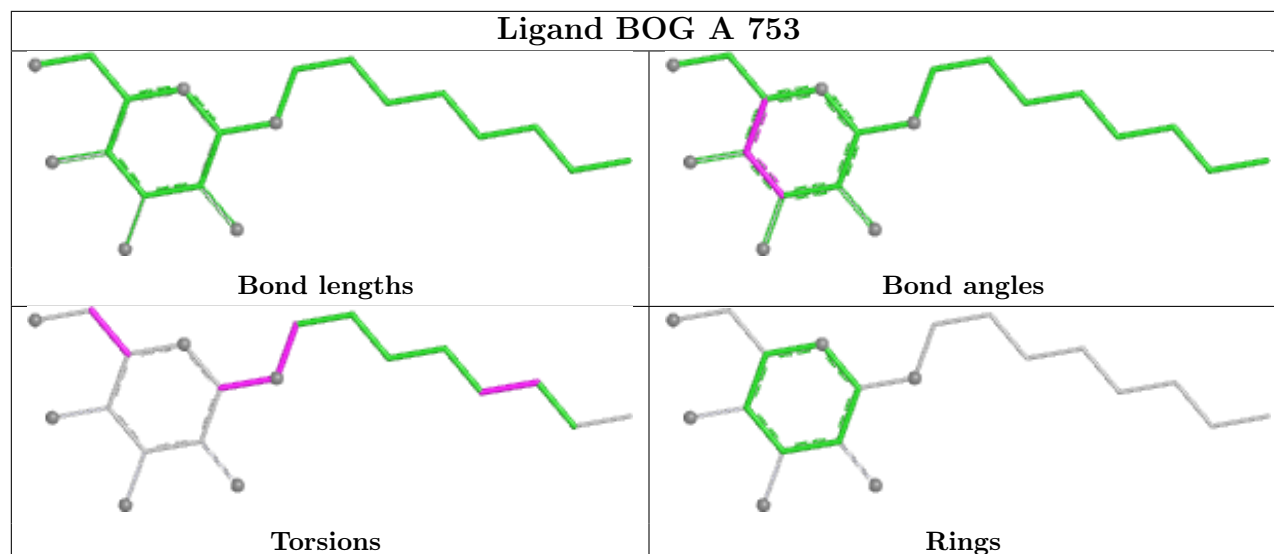
There are no ring outliers.

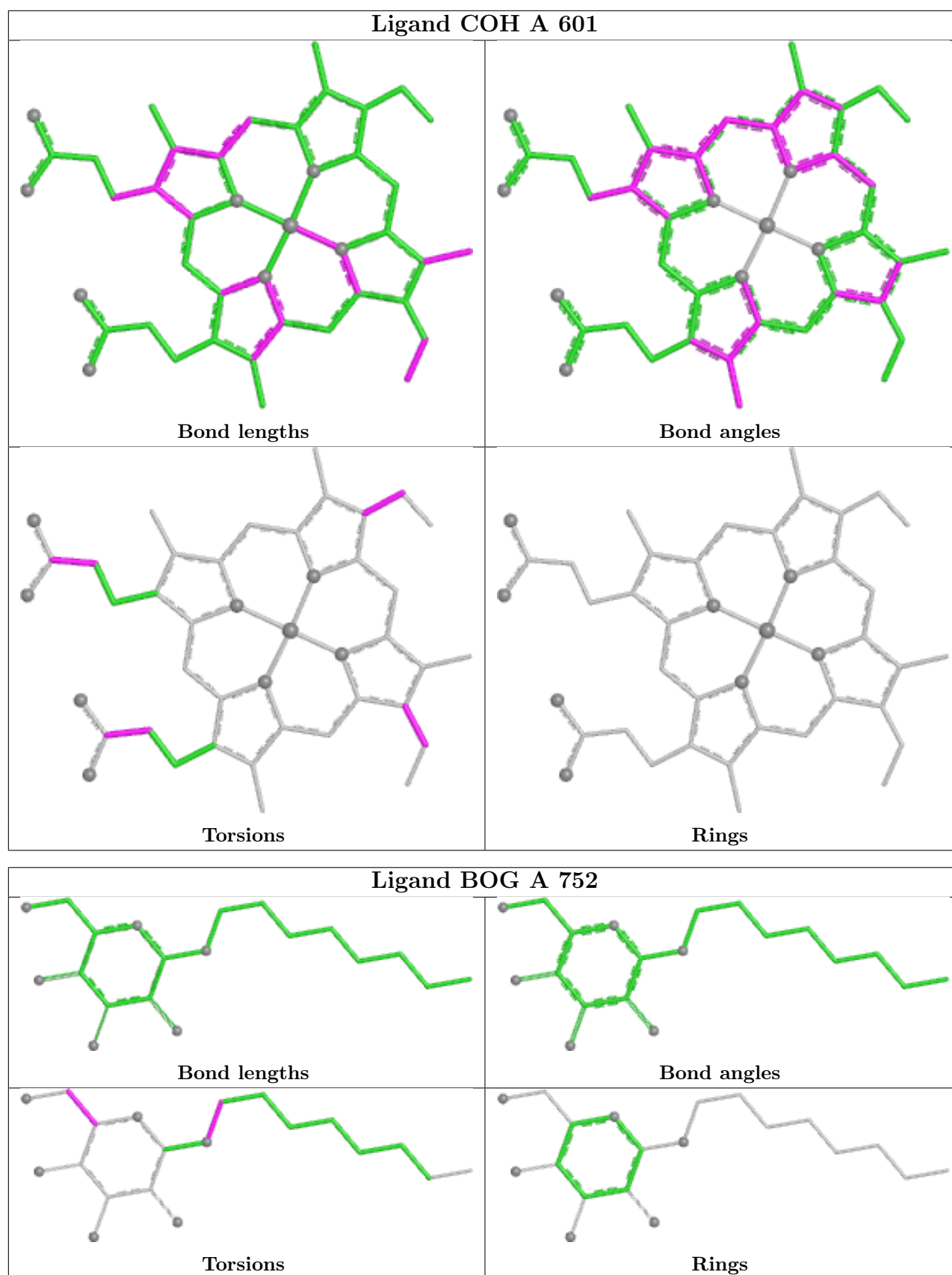
6 monomers are involved in 22 short contacts:

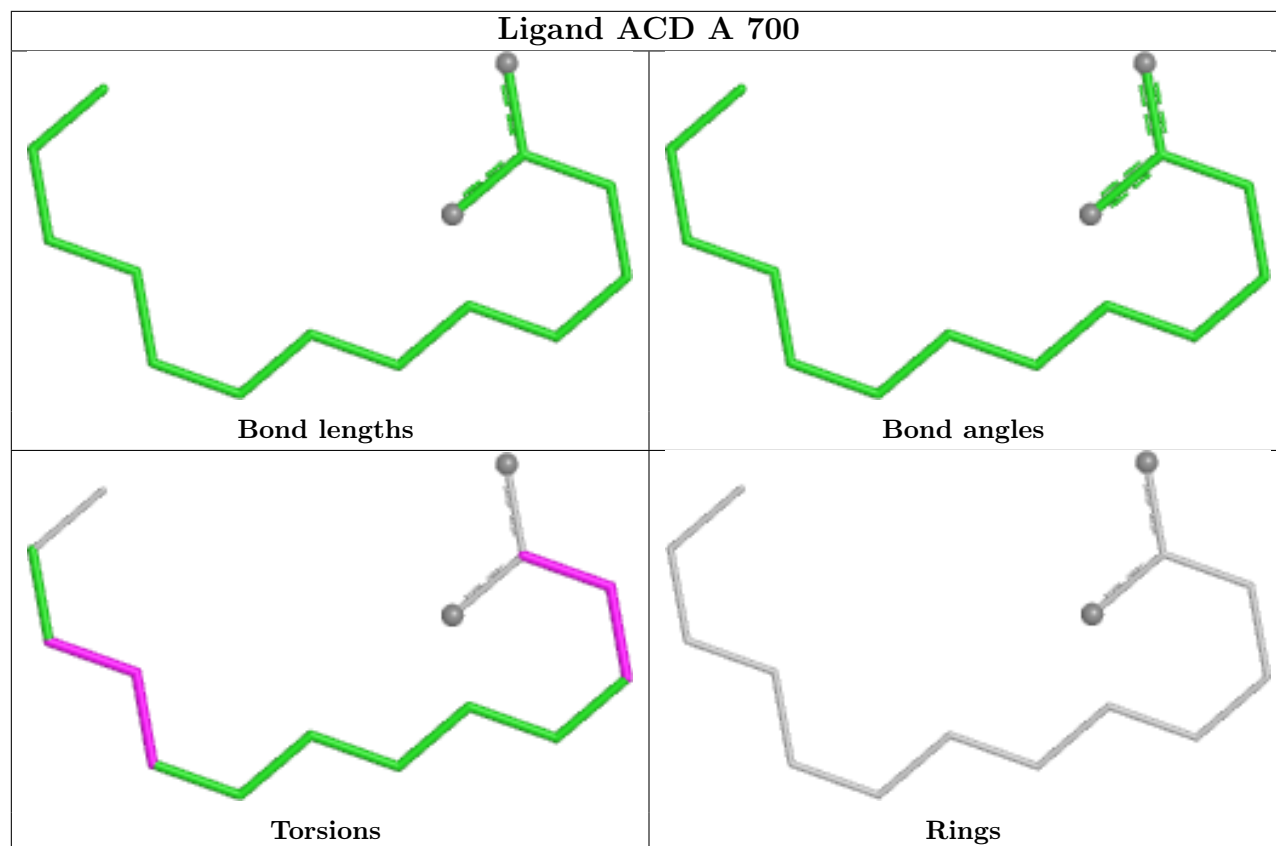
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	751	BOG	5	0
4	A	753	BOG	3	0
4	A	750	BOG	1	0
5	A	601	COH	2	0
4	A	752	BOG	4	0
6	A	700	ACD	7	0

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, 95th 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 ²)	Q<0.9
1	A	553/600 (92%)	-0.27	4 (0%) 84 68	20, 37, 70, 137	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	PRO	3.7
1	A	223	ALA	3.0
1	A	281	PRO	3.0
1	A	283	SER	2.7

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

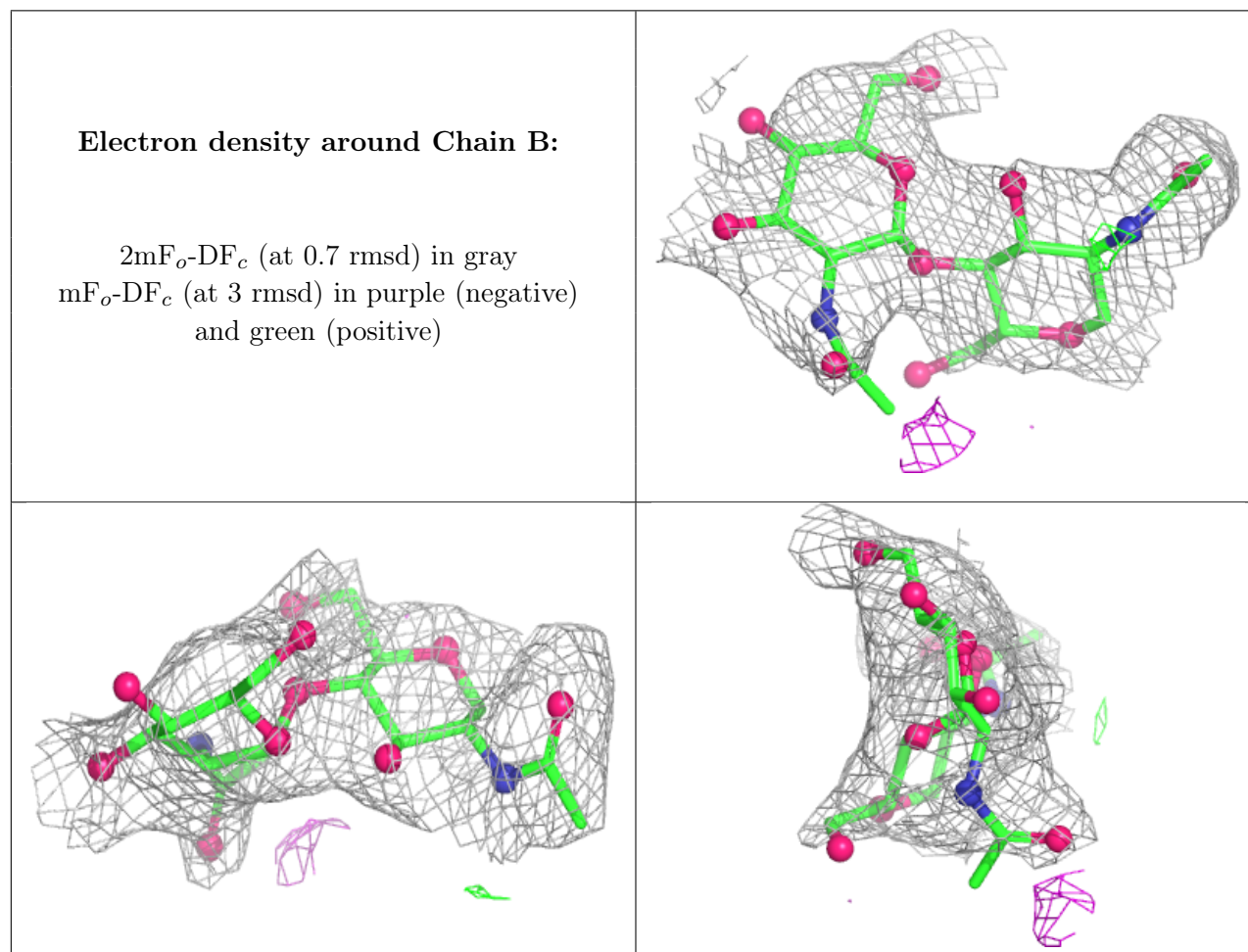
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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.

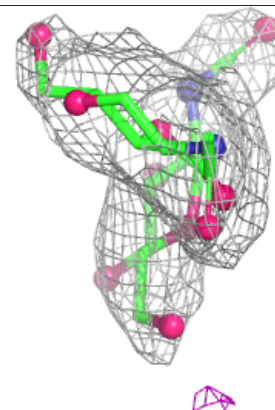
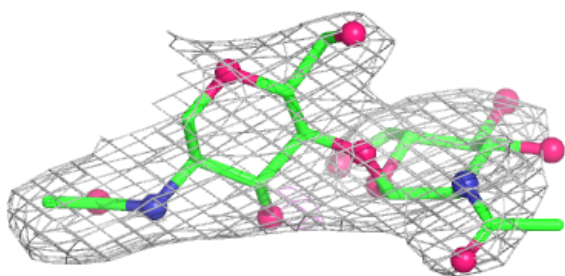
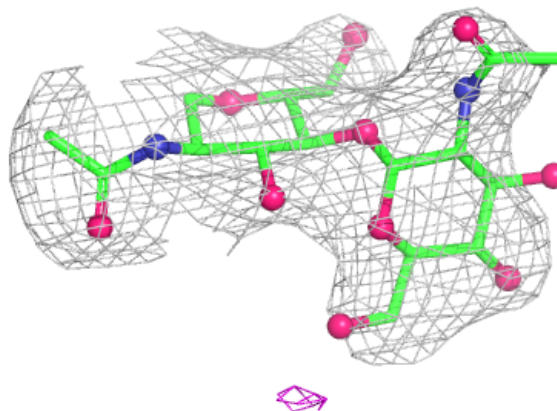
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	C	3	11/12	0.70	0.13	110,110,110,110	0
2	NDG	D	2	14/15	0.74	0.13	97,97,97,97	0
3	BMA	C	4	11/12	0.78	0.15	106,106,106,106	0
2	NAG	B	1	14/15	0.81	0.12	73,73,73,73	0
3	NAG	C	2	14/15	0.82	0.14	56,56,56,56	0
2	NAG	D	1	14/15	0.83	0.11	55,55,55,55	0
2	NDG	B	2	14/15	0.84	0.13	94,94,94,94	0
3	NAG	C	1	14/15	0.92	0.08	39,39,39,39	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.

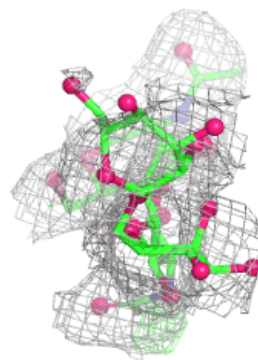
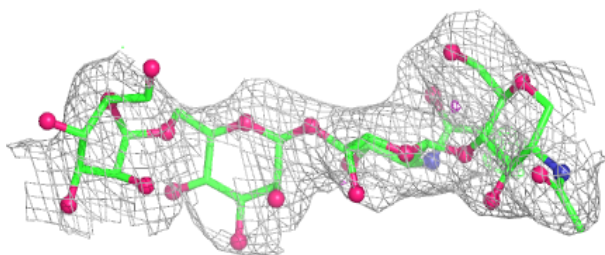
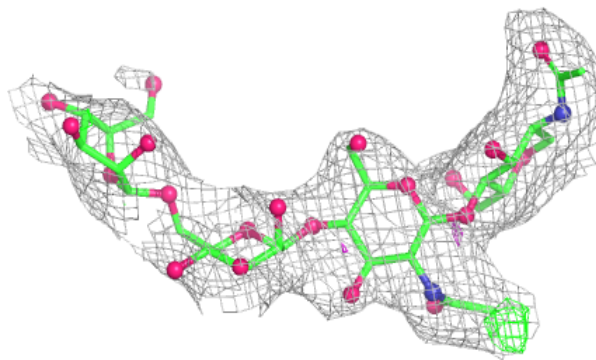


Electron density around Chain D:

$2mF_o-DF_c$ (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)



6.4 Ligands ⓘ

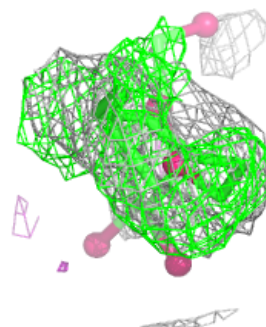
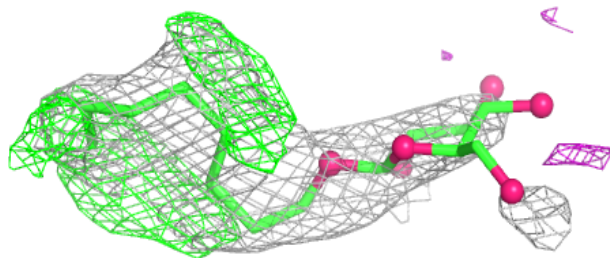
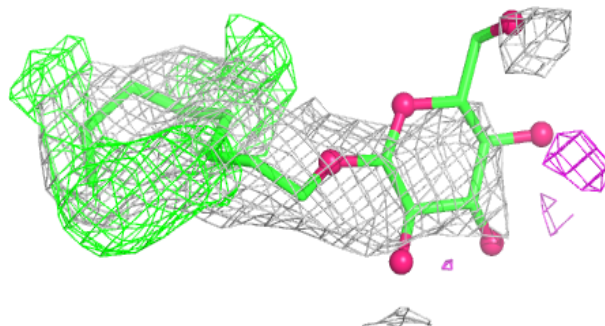
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BOG	A	753	20/20	0.33	0.42	63,63,63,63	20
4	BOG	A	752	20/20	0.71	0.18	60,60,60,60	0
5	COH	A	601	43/43	0.79	0.27	67,67,67,67	43
6	ACD	A	700	15/22	0.86	0.18	56,56,56,56	0
4	BOG	A	750	20/20	0.90	0.11	62,62,62,62	0
4	BOG	A	751	20/20	0.92	0.10	33,33,33,33	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.

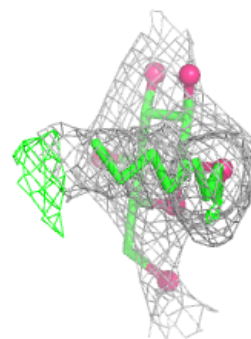
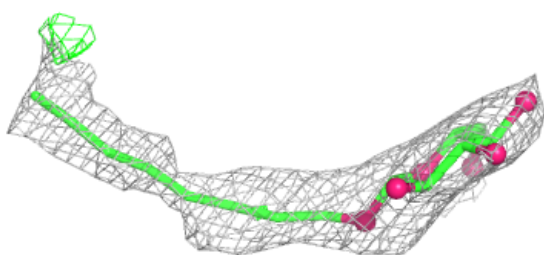
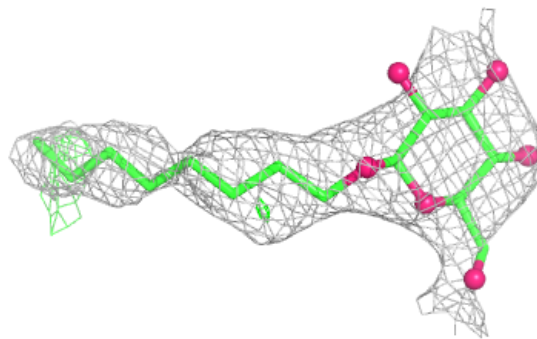
Electron density around BOG A 753:

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



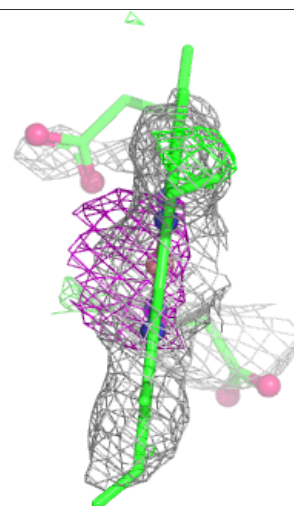
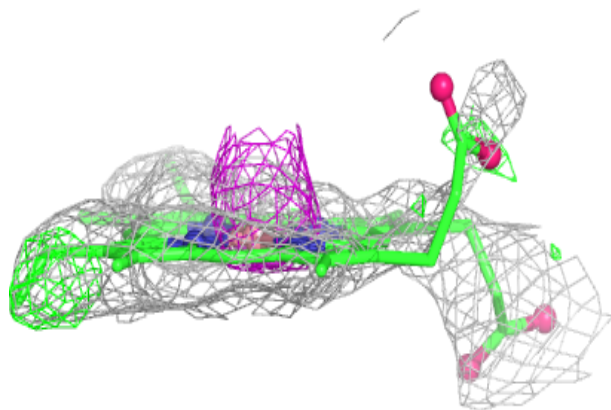
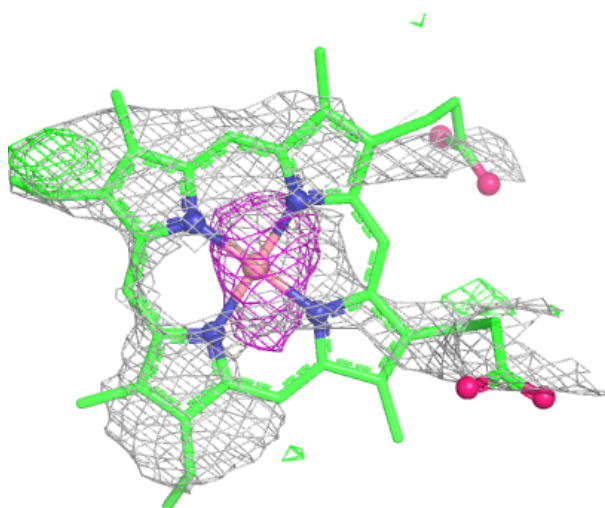
Electron density around BOG A 752:

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



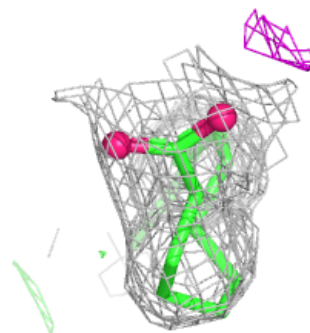
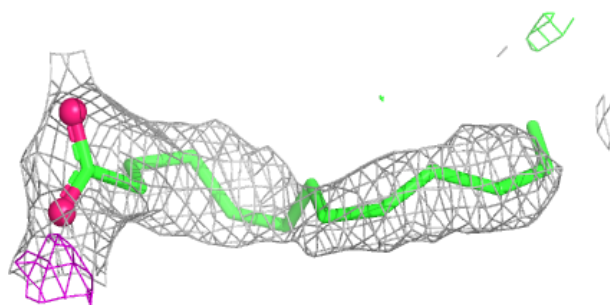
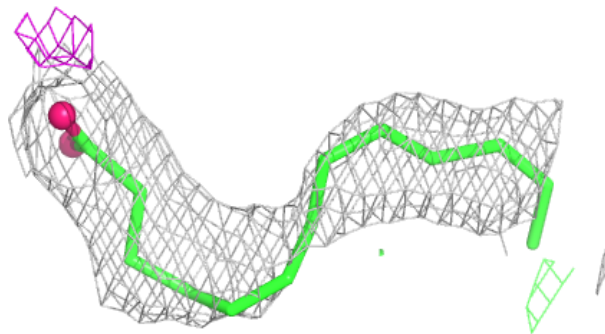
Electron density around COH A 601:

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

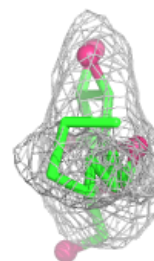
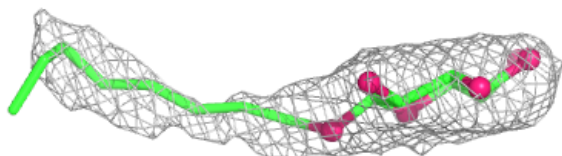
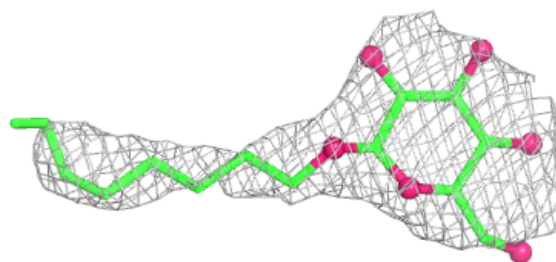


Electron density around ACD A 700:

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

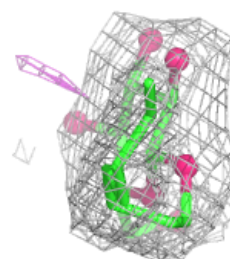
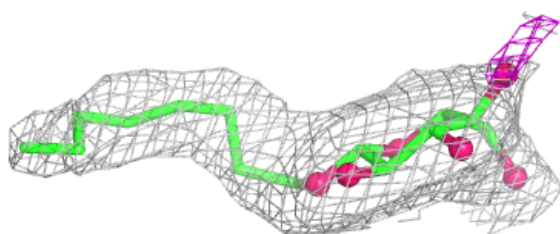
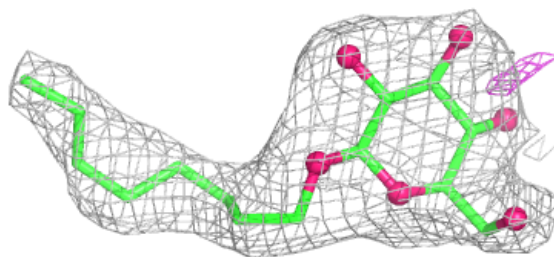
**Electron density around BOG A 750:**

$2mF_o-DF_c$ (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.