



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 1X38 / pdb_00001x38
Title : crystal structure of barley beta-D-glucan glucohydrolase isoenzyme exo1 in complex with gluco-phenylimidazole
Authors : Hrmova, M.; Streltsov, V.A.; Smith, B.J.; Vasella, A.; Varghese, J.N.; Fincher, G.B.
Deposited on : 2005-05-02
Resolution : 1.70 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

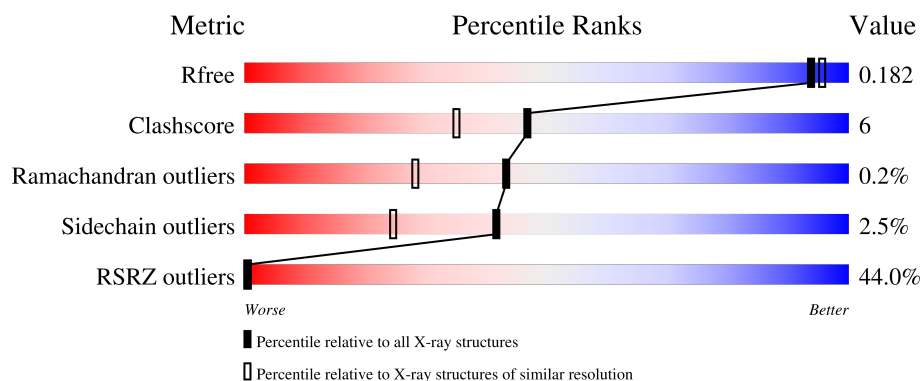
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	602	44% 91% 8%
2	B	3	33% 33% 33%
3	C	7	14% 57% 29%
4	D	5	80% 20%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5721 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.

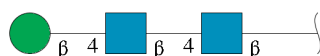
- Molecule 1 is a protein called beta-D-glucan exohydrolase isoenzyme ExoI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4566	2891	787	862	26	0	0	0

There is a discrepancy between the modelled and reference sequences:

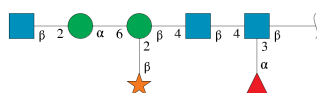
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	SEE REMARK 999	GB 4566505

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



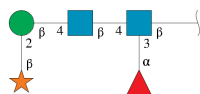
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-xylopyranose-(1-2)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



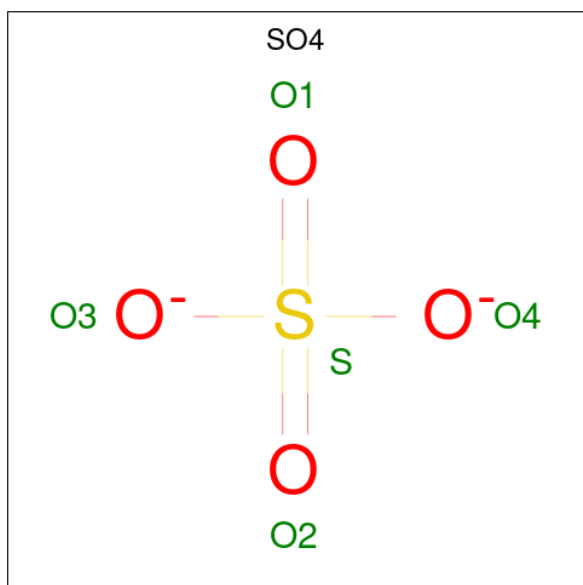
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	7	83	47	3	33	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



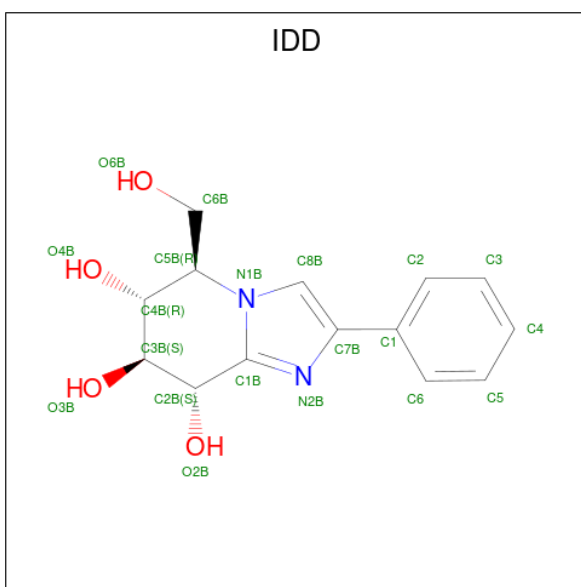
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			58	33	2	23			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (5R,6R,7S,8S)-5-(HYDROXYMETHYL)-2-PHENYL-5,6,7,8-TETRAHYDR OIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (CCD ID: IDD) (formula: C₁₄H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			7	3	4		
7	A	1	Total	C	O	0	1
			12	6	6		

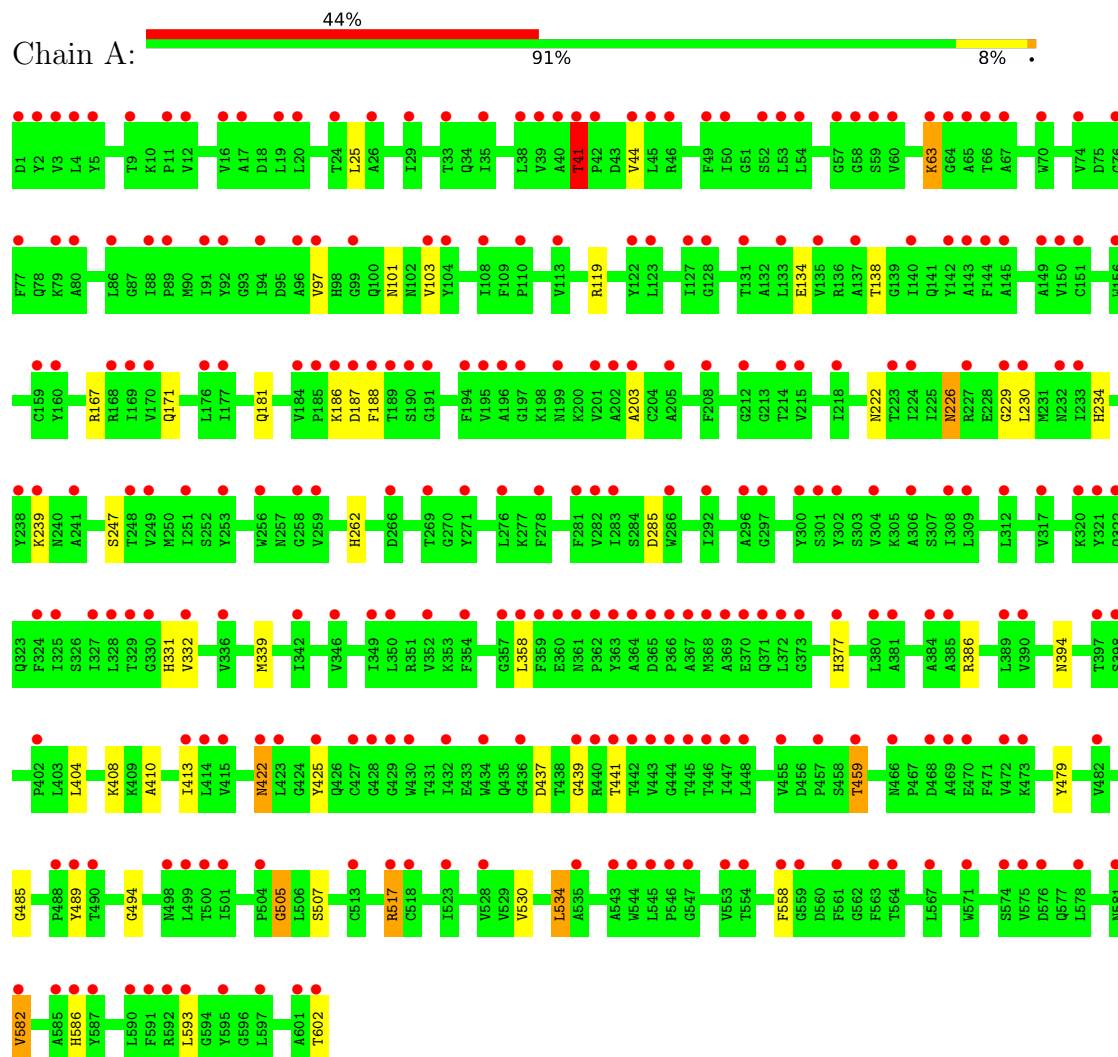
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	931	Total 931	O 931	0	0

3 Residue-property plots [i](#)

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: beta-D-glucan exohydrolase isoenzyme ExoI



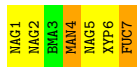
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-xylopyranose-(1-2)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 14% 57% 29%



- Molecule 4: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.56Å 100.56Å 182.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 – 1.70 34.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.30-1.70) 99.8 (34.30-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, R_{free}	0.160 , 0.183 0.158 , 0.182	Depositor DCC
R_{free} test set	5168 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5721	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GOL, XYP, IDD, MAN, NAG, SO4, FUC

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	0.64	0/4663	0.77	3/6334 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	THR	N-CA-CB	-5.39	103.65	111.25
1	A	485	GLY	N-CA-C	5.32	117.09	110.29
1	A	188	PHE	N-CA-C	5.20	117.84	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4566	0	4550	52	1
2	B	39	0	34	1	0
3	C	83	0	63	2	0
4	D	58	0	42	0	0
5	A	5	0	0	0	0
6	A	20	0	16	0	0
7	A	19	0	22	1	0
8	A	931	0	0	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5721	0	4727	54	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (54) 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:517:ARG:HB2	1:A:517:ARG:NH1	1.41	1.34
1:A:517:ARG:HH11	1:A:517:ARG:CB	1.47	1.27
1:A:41:THR:HG22	1:A:44:VAL:H	1.39	0.86
1:A:394:ASN:HD21	1:A:404:LEU:H	1.18	0.86
1:A:410:ALA:O	1:A:459:THR:HB	1.78	0.83
1:A:41:THR:HG21	8:A:6671:HOH:O	1.84	0.78
1:A:97:VAL:H	1:A:101:ASN:HD21	1.34	0.75
1:A:181:GLN:HE21	1:A:203:ALA:H	1.37	0.72
1:A:422:ASN:HD21	1:A:439:GLY:H	1.37	0.72
1:A:167:ARG:HH11	1:A:171:GLN:HE22	1.39	0.70
1:A:239:LYS:HE2	8:A:6936:HOH:O	1.91	0.70
1:A:505:GLY:N	8:A:6932:HOH:O	2.28	0.65
1:A:422:ASN:ND2	1:A:439:GLY:H	1.95	0.65
1:A:262:HIS:HE1	1:A:285:ASP:H	1.43	0.64
1:A:97:VAL:H	1:A:101:ASN:ND2	1.96	0.63
1:A:119:ARG:HE	7:A:2002[A]:GOL:H2	1.63	0.62
1:A:517:ARG:HB2	1:A:517:ARG:HH11	0.58	0.62
8:A:6766:HOH:O	3:C:7:FUC:H63	2.01	0.60
1:A:479:TYR:HB3	1:A:517:ARG:HH12	1.68	0.59
1:A:234:HIS:HE1	8:A:6196:HOH:O	1.86	0.58
1:A:386:ARG:NH1	8:A:6930:HOH:O	2.33	0.57
1:A:408:LYS:O	1:A:459:THR:HG21	2.04	0.57
1:A:167:ARG:NH1	1:A:171:GLN:HE22	2.02	0.56
1:A:167:ARG:HH11	1:A:171:GLN:NE2	2.01	0.56
1:A:234:HIS:HD2	8:A:6027:HOH:O	1.88	0.56
1:A:262:HIS:CE1	1:A:285:ASP:H	2.23	0.56
1:A:226:ASN:ND2	1:A:229:GLY:H	2.03	0.55
1:A:25:LEU:HD13	1:A:339:MET:HE1	1.89	0.55
1:A:331:HIS:HD2	8:A:6340:HOH:O	1.90	0.55
1:A:507:SER:OG	8:A:6932:HOH:O	2.18	0.54
1:A:422:ASN:HD22	1:A:422:ASN:C	2.16	0.54
1:A:582:VAL:HG11	1:A:593:LEU:HB3	1.89	0.54
1:A:181:GLN:HE22	1:A:247:SER:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HD3	1:A:186:LYS:H	1.75	0.52
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.94	0.51
1:A:530:VAL:HG13	1:A:534:LEU:HD22	1.92	0.51
1:A:226:ASN:C	1:A:226:ASN:HD22	2.19	0.51
1:A:41:THR:CG2	1:A:44:VAL:H	2.19	0.50
1:A:222:ASN:HB2	2:B:1:NAG:H82	1.96	0.48
1:A:437:ASP:HB3	1:A:441:THR:HG21	1.98	0.46
1:A:186:LYS:HD3	1:A:186:LYS:N	2.30	0.46
1:A:422:ASN:ND2	1:A:425:TYR:H	2.16	0.44
1:A:339:MET:HA	1:A:339:MET:HE2	1.99	0.44
1:A:332:VAL:HG11	1:A:339:MET:HE1	2.00	0.43
3:C:2:NAG:H82	3:C:4:MAN:O3	2.18	0.43
1:A:602:THR:HG21	8:A:6307:HOH:O	2.18	0.43
1:A:489:TYR:CD2	1:A:494:GLY:HA3	2.55	0.42
1:A:181:GLN:HE22	1:A:247:SER:N	2.18	0.42
1:A:63:LYS:N	1:A:63:LYS:HE3	2.35	0.42
1:A:558:PHE:HB2	8:A:6652:HOH:O	2.21	0.41
1:A:63:LYS:HE3	1:A:63:LYS:H	1.86	0.41
1:A:413:ILE:HG21	1:A:479:TYR:CZ	2.55	0.41
1:A:103:VAL:HG21	1:A:138:THR:HG21	2.03	0.40
1:A:186:LYS:H	1:A:186:LYS:CD	2.33	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LYS:NZ	8:A:6243:HOH:O[3_554]	2.09	0.11

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	600/602 (100%)	584 (97%)	15 (2%)	1 (0%)	43 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	485/485 (100%)	473 (98%)	12 (2%)	42 24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	63	LYS
1	A	187	ASP
1	A	226	ASN
1	A	230	LEU
1	A	358	LEU
1	A	422	ASN
1	A	459	THR
1	A	517	ARG
1	A	534	LEU
1	A	582	VAL
1	A	586	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	112	ASN
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	226	ASN
1	A	234	HIS
1	A	240	ASN
1	A	257	ASN
1	A	262	HIS
1	A	331	HIS
1	A	333	ASN
1	A	377	HIS
1	A	394	ASN
1	A	422	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 ⓘ

15 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	0.65	0	17,19,21	1.12	2 (11%)
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	0.77	0
2	BMA	B	3	2	11,11,12	0.63	0	15,15,17	0.93	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	1.06	0
3	BMA	C	3	3	11,11,12	0.56	0	15,15,17	0.64	0
3	MAN	C	4	3	11,11,12	0.54	0	15,15,17	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	5	3	14,14,15	0.42	0	17,19,21	0.89	1 (5%)
3	XYP	C	6	3	9,9,10	1.24	1 (11%)	10,12,14	0.67	0
3	FUC	C	7	3	10,10,11	0.59	0	14,14,16	0.81	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.58	0	17,19,21	0.80	0
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	0.54	0
4	BMA	D	3	4	11,11,12	0.54	0	15,15,17	0.66	0
4	XYP	D	4	4	9,9,10	1.23	1 (11%)	10,12,14	0.98	1 (10%)
4	FUC	D	5	4	10,10,11	0.57	0	14,14,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	XYP	C	6	3	-	-	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	XYP	D	4	4	-	-	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	XYP	O5-C1	-3.33	1.36	1.43
3	C	6	XYP	O5-C1	-3.29	1.36	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	XYP	C5-O5-C1	2.82	115.96	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.79	115.93	112.19
3	C	5	NAG	C1-O5-C5	2.74	115.85	112.19
2	B	1	NAG	O5-C1-C2	-2.60	107.27	111.29
3	C	7	FUC	O5-C5-C6	2.34	112.49	107.40
3	C	4	MAN	C1-O5-C5	2.18	115.10	112.19
2	B	3	BMA	C3-C4-C5	2.17	114.17	110.23
3	C	1	NAG	O5-C1-C2	-2.04	108.13	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

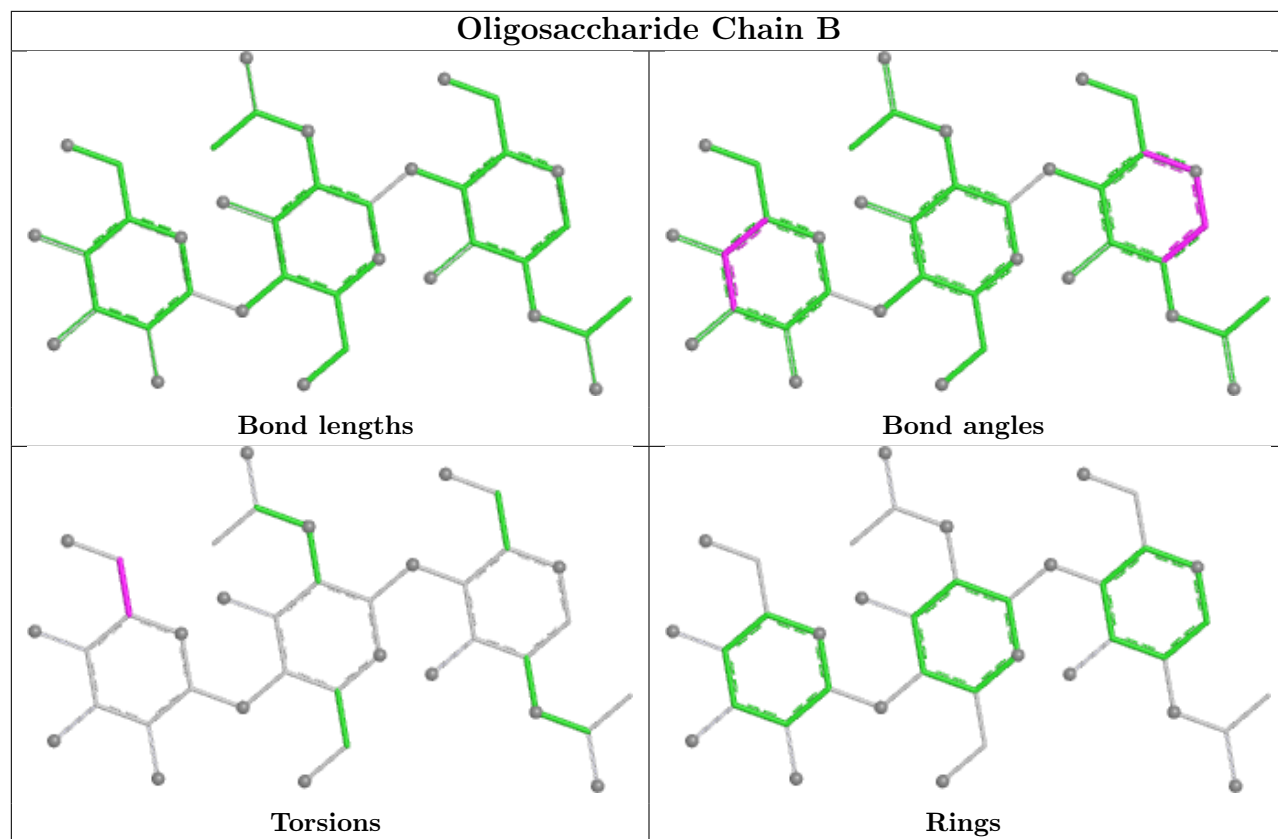
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

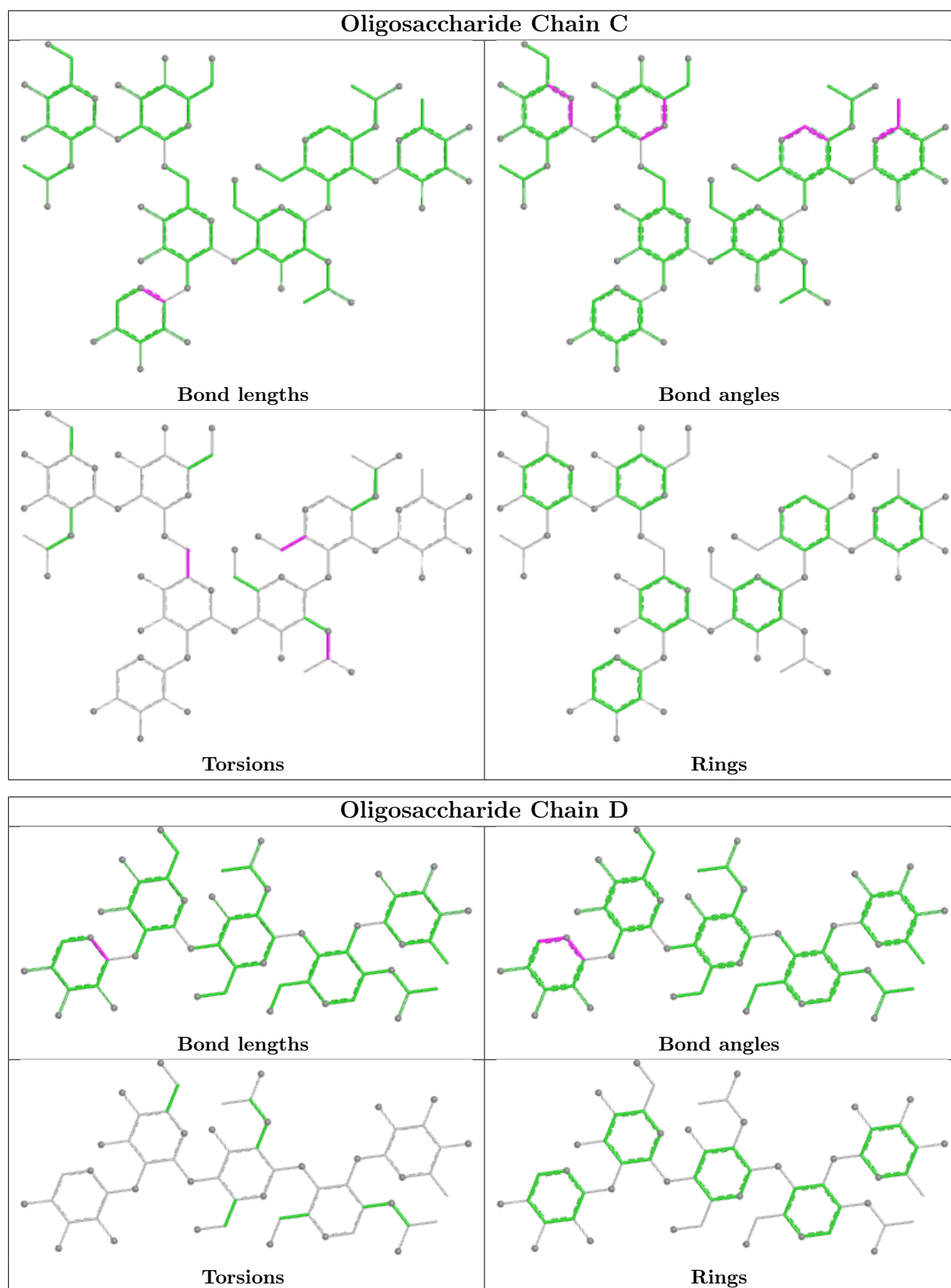
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	1	0
3	C	7	FUC	1	0
3	C	2	NAG	1	0
2	B	1	NAG	1	0

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





5.6 Ligand geometry

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
6	IDD	A	1001	-	21,22,22	0.97	0	23,32,32	1.76	6 (26%)
5	SO4	A	3001	-	4,4,4	0.27	0	6,6,6	0.21	0
7	GOL	A	2001[A]	-	5,5,5	0.53	0	5,5,5	0.35	0
7	GOL	A	2002[A]	-	5,5,5	0.44	0	5,5,5	0.23	0
7	GOL	A	2001[B]	-	5,5,5	0.54	0	5,5,5	0.27	0
7	GOL	A	2002[B]	-	5,5,5	0.34	0	5,5,5	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IDD	A	1001	-	-	0/6/26/26	0/3/3/3
7	GOL	A	2001[A]	-	-	0/4/4/4	-
7	GOL	A	2002[A]	-	-	2/4/4/4	-
7	GOL	A	2001[B]	-	-	2/4/4/4	-
7	GOL	A	2002[B]	-	-	2/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	IDD	C7B-C8B-N1B	-3.69	102.93	106.77
6	A	1001	IDD	C1-C7B-C8B	-3.65	124.07	129.65
6	A	1001	IDD	C1-C7B-N2B	3.32	125.03	119.95
6	A	1001	IDD	C2-C1-C7B	-3.11	117.39	120.87
6	A	1001	IDD	C8B-N1B-C1B	2.81	110.55	107.96
6	A	1001	IDD	C7B-N2B-C1B	2.13	107.47	105.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

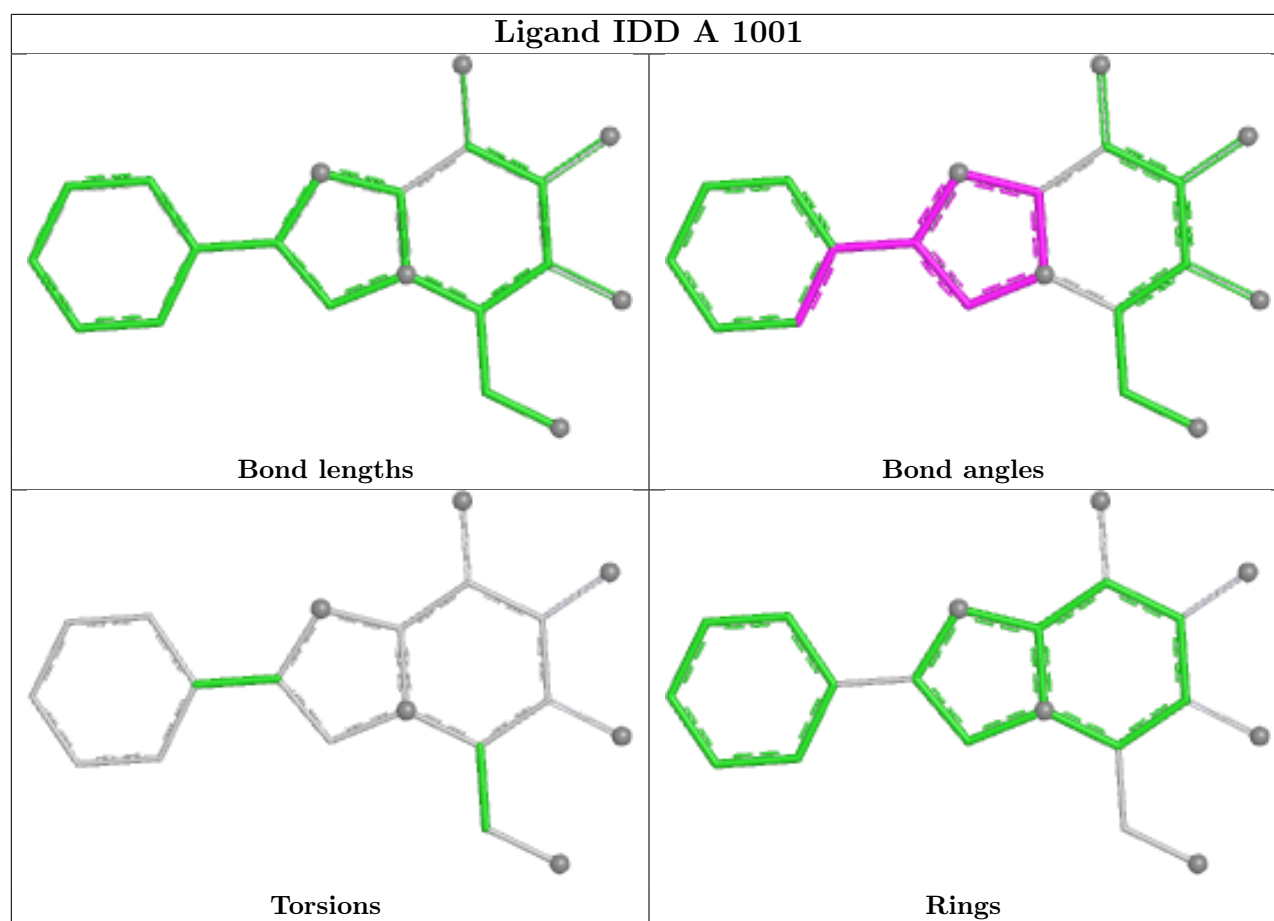
Mol	Chain	Res	Type	Atoms
7	A	2001[B]	GOL	O1-C1-C2-C3
7	A	2002[A]	GOL	O1-C1-C2-O2
7	A	2002[A]	GOL	O1-C1-C2-C3
7	A	2002[B]	GOL	O1-C1-C2-C3
7	A	2002[B]	GOL	O1-C1-C2-O2
7	A	2001[B]	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002[A]	GOL	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	602/602 (100%)	1.97	265 (44%) 0 0	22, 36, 43, 54	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	586	HIS	8.1
1	A	602	THR	5.8
1	A	187	ASP	5.1
1	A	582	VAL	4.6
1	A	63	LYS	4.5
1	A	186	LYS	4.3
1	A	1	ASP	4.2
1	A	214	THR	4.1
1	A	3	VAL	4.1
1	A	41	THR	4.0
1	A	498	ASN	4.0
1	A	432	ILE	3.8
1	A	233	ILE	3.7
1	A	370	GLU	3.7
1	A	2	TYR	3.7
1	A	45	LEU	3.6
1	A	517	ARG	3.5
1	A	44	VAL	3.5
1	A	188	PHE	3.4
1	A	373	GLY	3.4
1	A	322	GLN	3.3
1	A	26	ALA	3.3
1	A	601	ALA	3.3
1	A	430	TRP	3.3
1	A	159	CYS	3.2
1	A	576	ASP	3.2
1	A	327	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	359	PHE	3.2
1	A	363	TYR	3.2
1	A	140	ILE	3.2
1	A	4	LEU	3.1
1	A	561	PHE	3.1
1	A	74	VAL	3.1
1	A	92	TYR	3.1
1	A	76	GLY	3.1
1	A	585	ALA	3.1
1	A	103	VAL	3.1
1	A	122	TYR	3.1
1	A	380	LEU	3.1
1	A	77	PHE	3.1
1	A	317	VAL	3.0
1	A	19	LEU	3.0
1	A	53	LEU	3.0
1	A	54	LEU	3.0
1	A	42	PRO	3.0
1	A	321	TYR	3.0
1	A	88	ILE	3.0
1	A	367	ALA	3.0
1	A	320	LYS	3.0
1	A	466	ASN	3.0
1	A	332	VAL	3.0
1	A	5	TYR	3.0
1	A	20	LEU	3.0
1	A	86	LEU	3.0
1	A	368	MET	3.0
1	A	232	ASN	3.0
1	A	135	VAL	2.9
1	A	443	VAL	2.9
1	A	455	VAL	2.9
1	A	283	ILE	2.9
1	A	144	PHE	2.9
1	A	500	THR	2.9
1	A	385	ALA	2.9
1	A	504	PRO	2.9
1	A	49	PHE	2.9
1	A	60	VAL	2.9
1	A	201	VAL	2.9
1	A	302	TYR	2.9
1	A	545	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	2.8
1	A	184	VAL	2.8
1	A	271	TYR	2.8
1	A	366	PRO	2.8
1	A	398	SER	2.8
1	A	364	ALA	2.8
1	A	384	ALA	2.8
1	A	215	VAL	2.8
1	A	336	VAL	2.8
1	A	195	VAL	2.8
1	A	362	PRO	2.8
1	A	300	TYR	2.8
1	A	46	ARG	2.7
1	A	448	LEU	2.7
1	A	439	GLY	2.7
1	A	518	CYS	2.7
1	A	79	LYS	2.7
1	A	473	LYS	2.7
1	A	137	ALA	2.7
1	A	306	ALA	2.7
1	A	381	ALA	2.7
1	A	194	PHE	2.7
1	A	113	VAL	2.7
1	A	346	VAL	2.7
1	A	361	ASN	2.7
1	A	429	GLY	2.7
1	A	169	ILE	2.7
1	A	349	ILE	2.7
1	A	442	THR	2.6
1	A	224	ILE	2.6
1	A	38	LEU	2.6
1	A	513	CYS	2.6
1	A	156	TRP	2.6
1	A	145	ALA	2.6
1	A	189	THR	2.6
1	A	230	LEU	2.6
1	A	350	LEU	2.6
1	A	142	TYR	2.6
1	A	304	VAL	2.6
1	A	52	SER	2.6
1	A	199	ASN	2.6
1	A	434	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	278	PHE	2.5
1	A	259	VAL	2.5
1	A	440	ARG	2.5
1	A	553	VAL	2.5
1	A	428	GLY	2.5
1	A	24	THR	2.5
1	A	544	TRP	2.5
1	A	276	LEU	2.5
1	A	389	LEU	2.5
1	A	104	TYR	2.5
1	A	12	VAL	2.5
1	A	50	ILE	2.5
1	A	80	ALA	2.5
1	A	108	ILE	2.5
1	A	325	ILE	2.5
1	A	397	THR	2.5
1	A	70	TRP	2.5
1	A	593	LEU	2.5
1	A	40	ALA	2.5
1	A	149	ALA	2.5
1	A	91	ILE	2.5
1	A	523	ILE	2.5
1	A	468	ASP	2.4
1	A	312	LEU	2.4
1	A	423	LEU	2.4
1	A	578	LEU	2.4
1	A	258	GLY	2.4
1	A	65	ALA	2.4
1	A	238	TYR	2.4
1	A	66	THR	2.4
1	A	170	VAL	2.4
1	A	390	VAL	2.4
1	A	447	ILE	2.4
1	A	365	ASP	2.4
1	A	427	CYS	2.4
1	A	372	LEU	2.4
1	A	547	GLY	2.4
1	A	546	PRO	2.4
1	A	324	PHE	2.4
1	A	196	ALA	2.4
1	A	564	THR	2.4
1	A	457	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	358	LEU	2.4
1	A	469	ALA	2.4
1	A	281	PHE	2.4
1	A	490	THR	2.4
1	A	168	ARG	2.4
1	A	415	VAL	2.4
1	A	64	GLY	2.3
1	A	212	GLY	2.3
1	A	229	GLY	2.3
1	A	297	GLY	2.3
1	A	357	GLY	2.3
1	A	241	ALA	2.3
1	A	543	ALA	2.3
1	A	554	THR	2.3
1	A	208	PHE	2.3
1	A	354	PHE	2.3
1	A	571	TRP	2.3
1	A	35	ILE	2.3
1	A	94	ILE	2.3
1	A	150	VAL	2.3
1	A	352	VAL	2.3
1	A	190	SER	2.3
1	A	99	GLY	2.3
1	A	197	GLY	2.3
1	A	110	PRO	2.3
1	A	67	ALA	2.3
1	A	123	LEU	2.3
1	A	176	LEU	2.3
1	A	309	LEU	2.3
1	A	597	LEU	2.3
1	A	482	VAL	2.3
1	A	528	VAL	2.3
1	A	330	GLY	2.3
1	A	185	PRO	2.3
1	A	445	THR	2.3
1	A	446	THR	2.3
1	A	369	ALA	2.3
1	A	328	LEU	2.3
1	A	590	LEU	2.3
1	A	470	GLU	2.3
1	A	227	ARG	2.3
1	A	574	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	592	ARG	2.3
1	A	425	TYR	2.3
1	A	595	TYR	2.3
1	A	58	GLY	2.3
1	A	342	ILE	2.3
1	A	11	PRO	2.2
1	A	131	THR	2.2
1	A	329	THR	2.2
1	A	202	ALA	2.2
1	A	191	GLY	2.2
1	A	559	GLY	2.2
1	A	489	TYR	2.2
1	A	472	VAL	2.2
1	A	256	TRP	2.2
1	A	203	ALA	2.2
1	A	414	LEU	2.2
1	A	591	PHE	2.2
1	A	160	TYR	2.2
1	A	127	ILE	2.2
1	A	177	ILE	2.2
1	A	218	ILE	2.2
1	A	9	THR	2.2
1	A	269	THR	2.2
1	A	422	ASN	2.2
1	A	459	THR	2.2
1	A	488	PRO	2.2
1	A	535	ALA	2.2
1	A	286	TRP	2.2
1	A	360	GLU	2.2
1	A	57	GLY	2.2
1	A	436	GLY	2.2
1	A	444	GLY	2.2
1	A	558	PHE	2.2
1	A	29	ILE	2.2
1	A	402	PRO	2.2
1	A	266	ASP	2.1
1	A	39	VAL	2.1
1	A	205	ALA	2.1
1	A	296	ALA	2.1
1	A	248	THR	2.1
1	A	501	ILE	2.1
1	A	587	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	282	VAL	2.1
1	A	151	CYS	2.1
1	A	581	ASN	2.1
1	A	371	GLN	2.1
1	A	441	THR	2.1
1	A	251	ILE	2.1
1	A	413	ILE	2.1
1	A	377	HIS	2.1
1	A	249	VAL	2.1
1	A	59	SER	2.1
1	A	499	LEU	2.1
1	A	223	THR	2.1
1	A	89	PRO	2.1
1	A	292	ILE	2.1
1	A	308	ILE	2.1
1	A	128	GLY	2.0
1	A	17	ALA	2.0
1	A	143	ALA	2.0
1	A	301	SER	2.0
1	A	575	VAL	2.0
1	A	133	LEU	2.0
1	A	567	LEU	2.0
1	A	33	THR	2.0
1	A	253	TYR	2.0
1	A	563	PHE	2.0
1	A	96	ALA	2.0
1	A	97	VAL	2.0
1	A	239	LYS	2.0

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

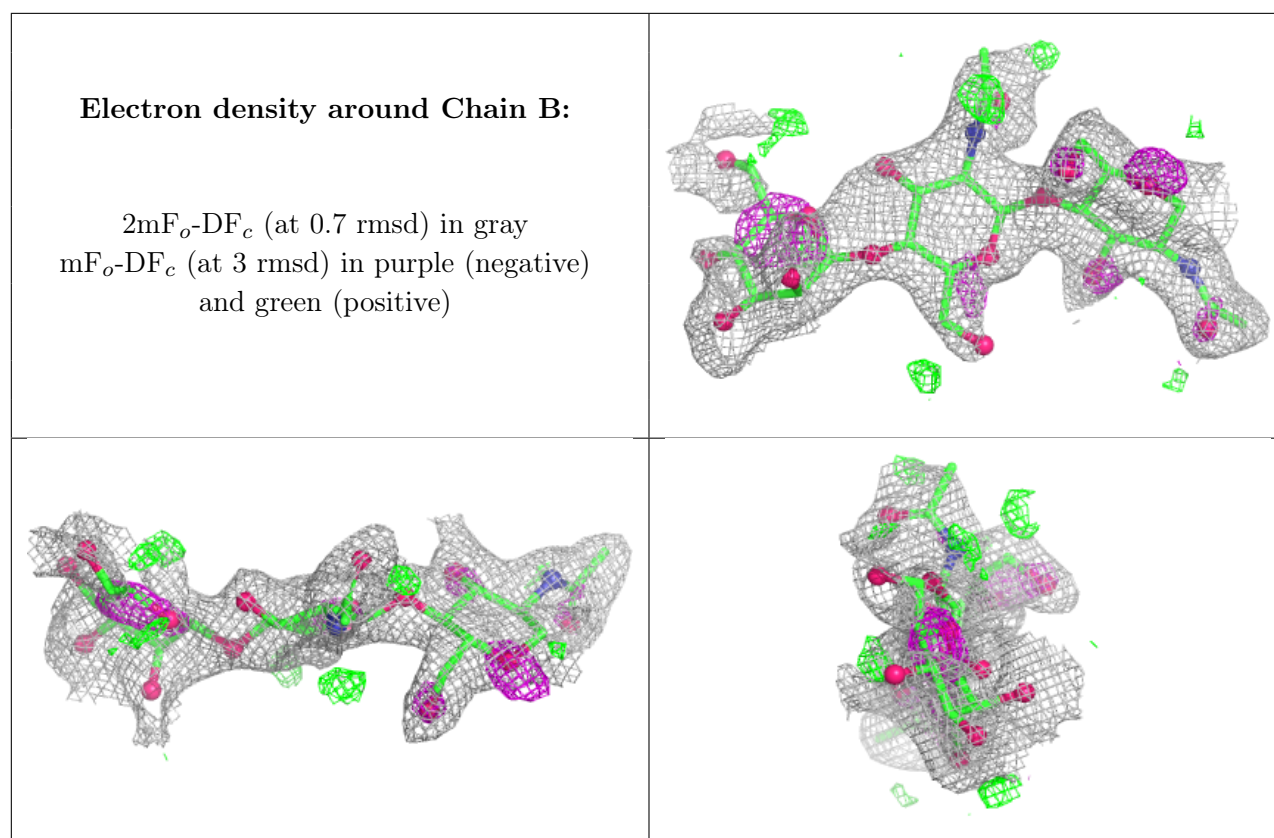
There are no non-standard protein/DNA/RNA residues in this entry.

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.

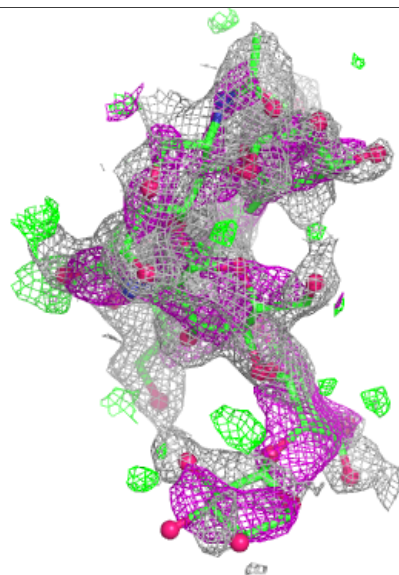
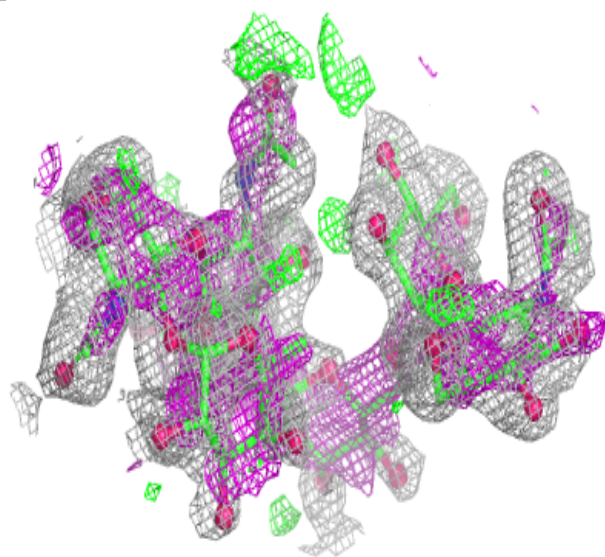
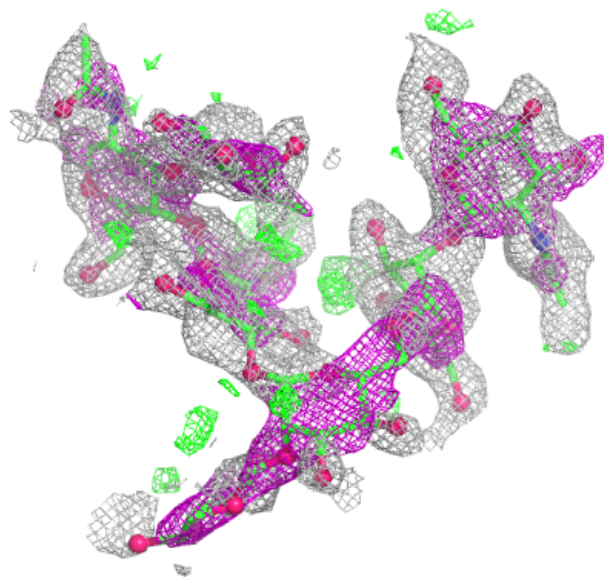
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XYP	C	6	9/10	-0.02	0.34	67,68,70,70	0
3	BMA	C	3	11/12	0.39	0.26	56,61,63,65	0
2	BMA	B	3	11/12	0.39	0.22	67,69,70,70	0
3	NAG	C	2	14/15	0.48	0.24	58,59,60,61	0
3	FUC	C	7	10/11	0.50	0.24	58,59,59,59	0
3	NAG	C	1	14/15	0.62	0.20	51,54,56,56	0
4	BMA	D	3	11/12	0.63	0.21	47,52,54,55	0
3	MAN	C	4	11/12	0.65	0.20	50,51,53,53	0
4	FUC	D	5	10/11	0.68	0.20	57,58,60,60	0
3	NAG	C	5	14/15	0.70	0.19	42,49,50,50	0
2	NAG	B	2	14/15	0.72	0.20	56,60,61,65	0
4	NAG	D	1	14/15	0.78	0.17	44,50,54,55	0
4	NAG	D	2	14/15	0.79	0.17	50,51,53,53	0
4	XYP	D	4	9/10	0.83	0.17	42,44,45,46	0
2	NAG	B	1	14/15	0.88	0.14	38,41,46,51	0

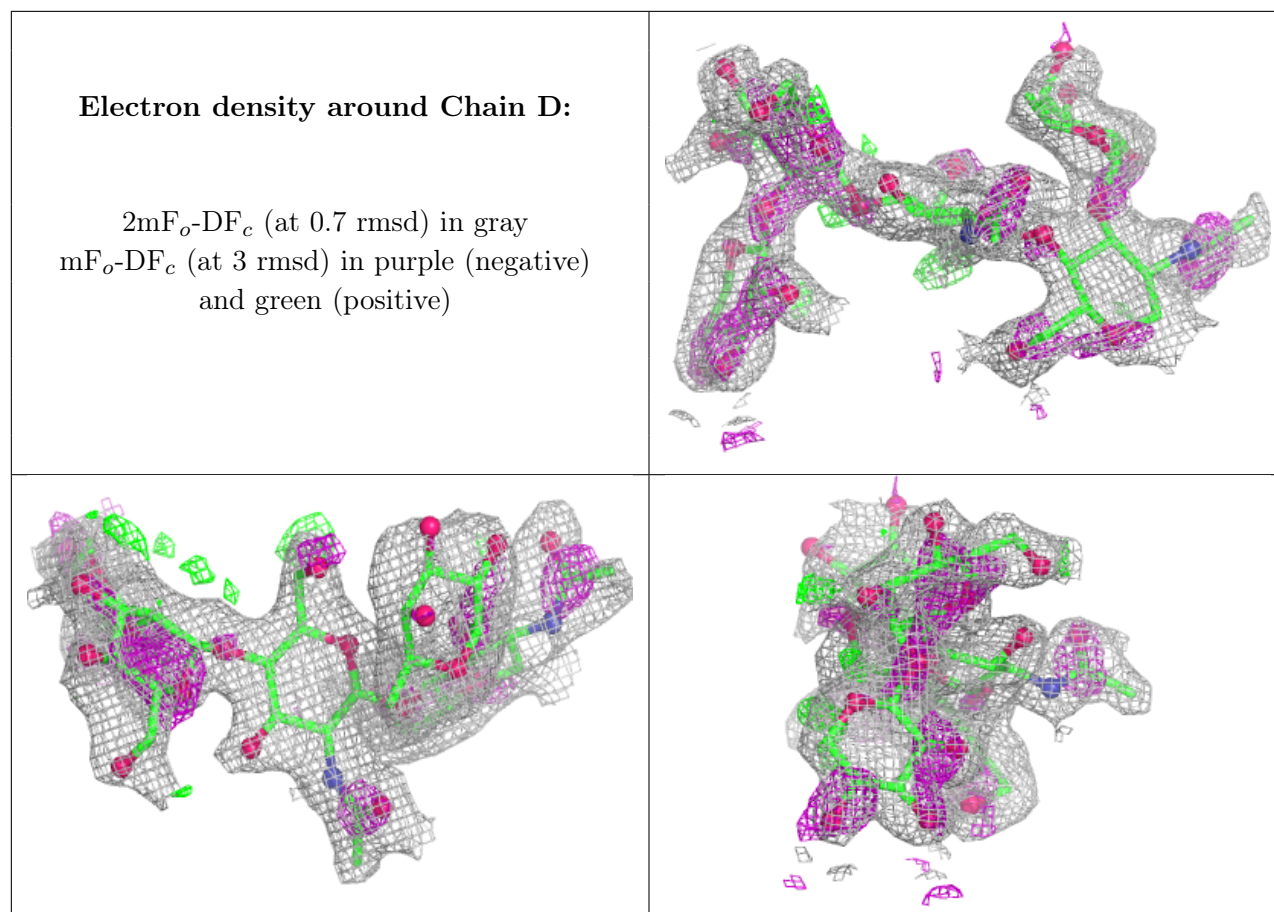
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

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



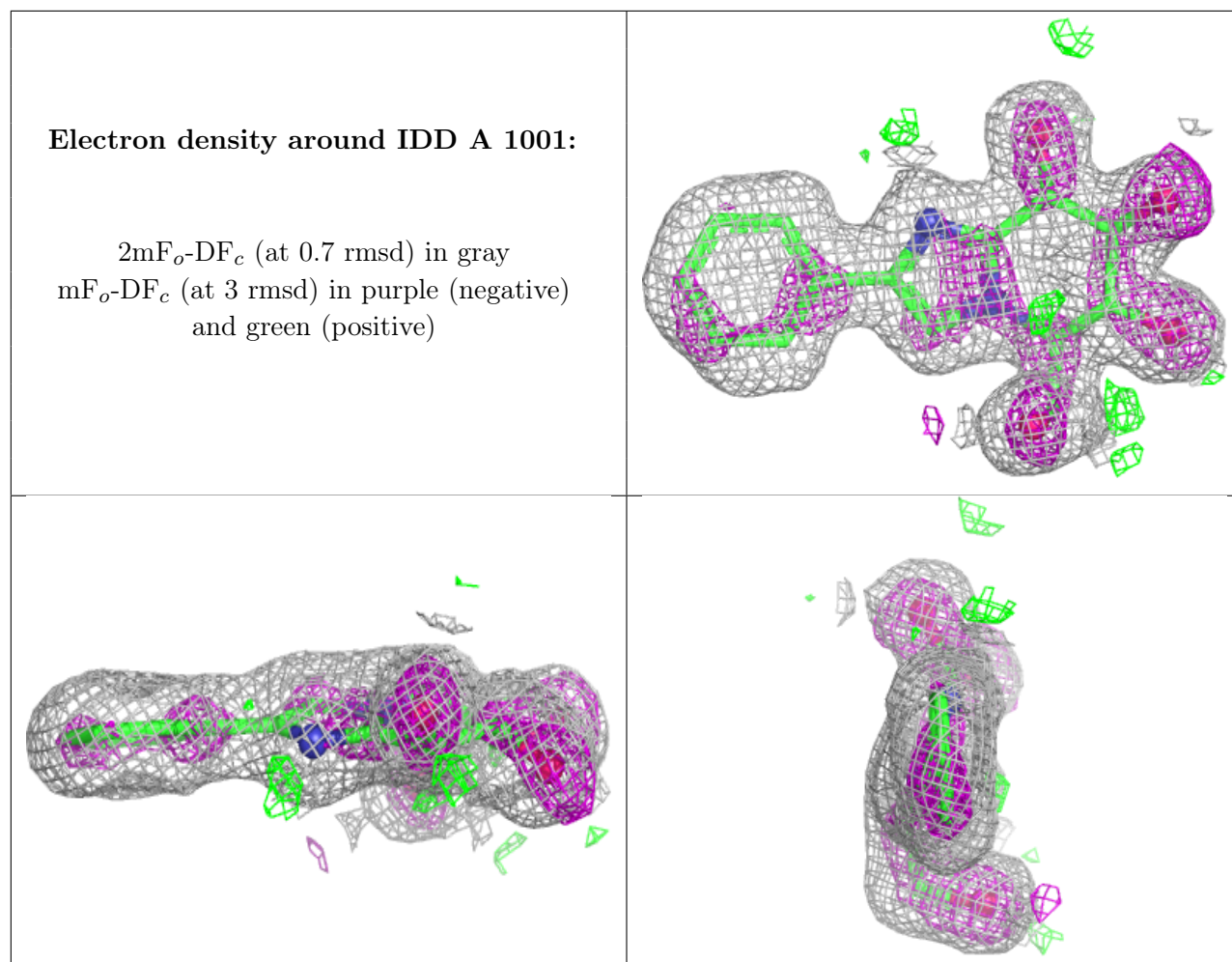


6.4 Ligands [i](#)

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
5	SO4	A	3001	5/5	0.66	0.20	61,62,63,63	0
7	GOL	A	2002[A]	6/6	0.68	0.21	37,40,40,40	6
7	GOL	A	2002[B]	6/6	0.68	0.21	39,39,39,41	6
7	GOL	A	2001[A]	6/6	0.86	0.15	25,32,37,40	1
7	GOL	A	2001[B]	6/6	0.86	0.15	32,33,37,40	1
6	IDD	A	1001	20/20	0.95	0.10	17,20,25,26	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.