Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:55 PM UTC

PDB ID	:	3D7F / pdb_00003d7f
Title	:	A high resolution crystal structure of human glutamate carboxypeptidase II (GCPII) in a complex with DCIT, a urea-based inhibitor
Authors	:	Lubkowski, J.; Barinka, C.
Deposited on	:	2008-05-21
Resolution	:	1.54 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:

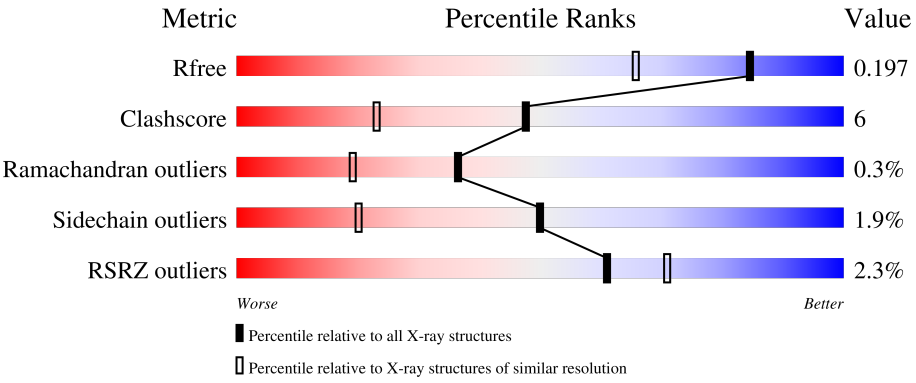
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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 <=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	709	2% 87% 10%
2	B	2	50% 50%
2	C	2	100%
3	D	3	33% 33% 33%
4	E	4	25% 75%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6603 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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	61	0
			5729	3687	951	1067	24			

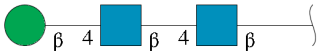
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609

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

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

- Molecule 3 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.

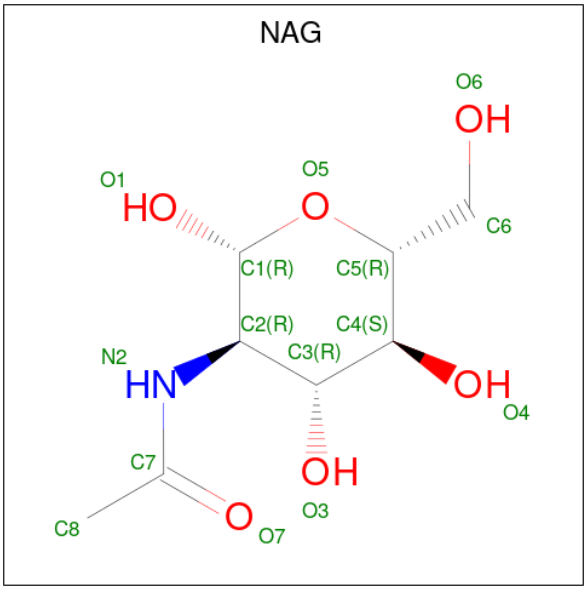


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	3	Total C N O 39 22 2 15	0	0	0

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0

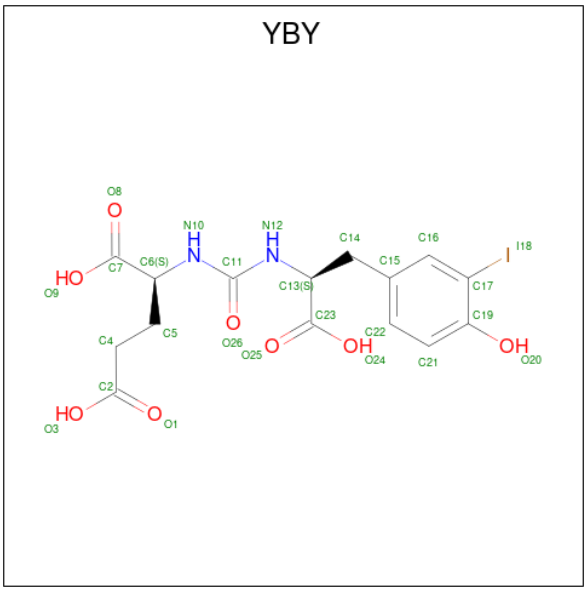
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is N-{[(1S)-1-carboxy-2-(4-hydroxy-3-iodophenyl)ethyl]carbamoyl}-L-glutamic acid (CCD ID: YBY) (formula: $C_{15}H_{17}IN_2O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C I N O 26 15 1 2 8	0	0

- Molecule 10 is water.

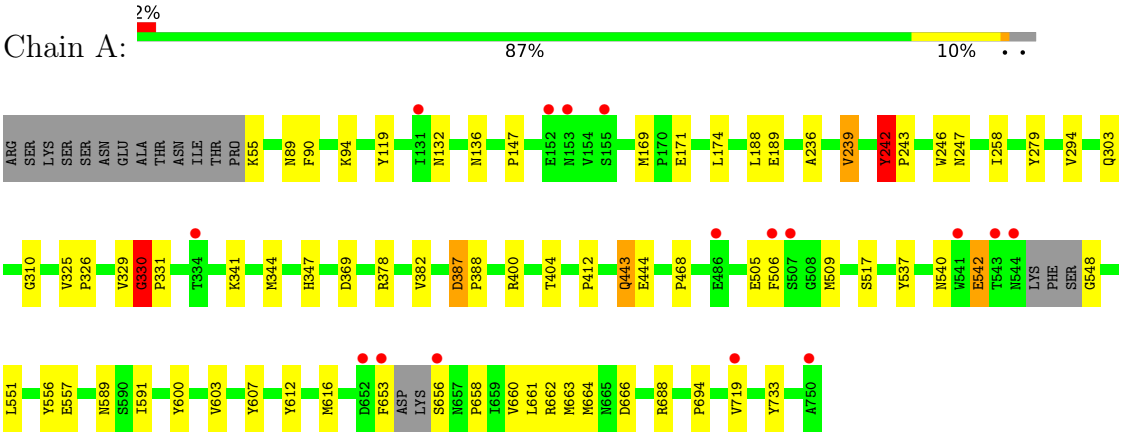
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	657	Total O 657 657	0	3

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: Glutamate carboxypeptidase 2

Chain A:

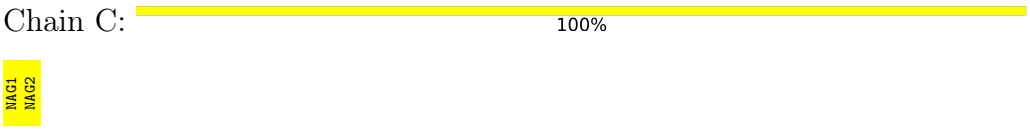


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

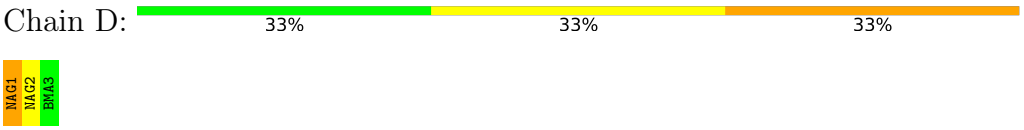
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



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

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.43Å 130.06Å 158.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.54 15.00 – 1.54	Depositor EDS
% Data completeness (in resolution range)	94.6 (15.00-1.54) 94.4 (15.00-1.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.195 0.178 , 0.197	Depositor DCC
R_{free} test set	1447 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6603	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: YBY, NAG, ZN, CL, BMA, CA, 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	1.00	0/6112	1.05	7/8274 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	GLY	CA-C-N	9.27	131.43	119.84
1	A	330	GLY	C-N-CA	9.27	131.43	119.84
1	A	242	TYR	C-N-CD	-7.07	105.04	120.60
1	A	147	PRO	O-C-N	6.28	124.10	121.15
1	A	331	PRO	N-CA-C	-5.32	101.52	112.47
1	A	119	TYR	CA-C-N	-5.27	114.81	120.03
1	A	119	TYR	C-N-CA	-5.27	114.81	120.03

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	TYR	Mainchain,Peptide
1	A	330	GLY	Mainchain,Peptide
1	A	387	ASP	Mainchain

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	5729	0	5597	63	2
2	B	28	0	25	1	0
2	C	28	0	25	0	0
3	D	39	0	34	2	0
4	E	50	0	43	0	0
5	A	42	0	39	1	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	26	0	14	0	0
10	A	657	0	0	13	4
All	All	6603	0	5777	66	4

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 (66) 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:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.29	1.26
1:A:171[B]:GLU:CD	1:A:341[B]:LYS:HE3	1.87	1.00
1:A:89[B]:ASN:HD21	1:A:378:ARG:HH21	1.03	0.95
1:A:171[B]:GLU:OE2	1:A:341[B]:LYS:CE	2.17	0.93
1:A:658[A]:PRO:HB3	10:A:2128:HOH:O	1.74	0.87
1:A:171[B]:GLU:OE2	1:A:341[B]:LYS:HE3	1.72	0.87
1:A:89[B]:ASN:ND2	1:A:378:ARG:HH21	1.75	0.84
1:A:733:TYR:HE2	10:A:2147:HOH:O	1.60	0.83
1:A:242:TYR:OH	10:A:2416:HOH:O	2.01	0.78
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.83	0.77
1:A:540:ASN:OD1	1:A:542:GLU:HB3	1.85	0.75
1:A:171[B]:GLU:OE2	1:A:341[B]:LYS:NZ	2.19	0.75
1:A:89[B]:ASN:HD21	1:A:378:ARG:NH2	1.83	0.75
1:A:548:GLY:HA3	10:A:2387:HOH:O	1.87	0.74
1:A:188:LEU:HD11	1:A:329:VAL:HG11	1.74	0.70
1:A:603[B]:VAL:HG13	1:A:607:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90[B]:PHE:HE2	1:A:94:LYS:HZ3	1.41	0.68
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.25	0.65
1:A:603[B]:VAL:HG13	1:A:607:TYR:CZ	2.31	0.65
1:A:506:PHE:HB2	1:A:509:MET:HE2	1.82	0.62
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.39	0.58
1:A:603[B]:VAL:CG1	1:A:607:TYR:CE2	2.87	0.57
1:A:591[A]:ILE:HG23	1:A:661[A]:LEU:HD21	1.87	0.57
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.28	0.55
1:A:666:ASP:OD2	10:A:1986:HOH:O	2.18	0.55
1:A:188:LEU:HD11	1:A:329:VAL:CG1	2.38	0.52
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.90	0.52
1:A:661[A]:LEU:O	1:A:664[A]:MET:HB2	2.10	0.52
1:A:303:GLN:HE21	1:A:325:VAL:HG13	1.75	0.51
1:A:506:PHE:CB	1:A:509:MET:HE2	2.41	0.50
10:A:2019:HOH:O	2:B:2:NAG:H81	2.12	0.50
1:A:90[B]:PHE:CE2	1:A:94:LYS:NZ	2.77	0.50
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.92	0.50
1:A:246:TRP:CD1	5:A:1760:NAG:H83	2.48	0.49
1:A:169:MET:HE2	1:A:347:HIS:NE2	2.28	0.48
1:A:540:ASN:C	1:A:542:GLU:H	2.21	0.48
1:A:653:PHE:HZ	1:A:661[A]:LEU:HD13	1.78	0.48
1:A:310:GLY:O	1:A:330:GLY:HA2	2.14	0.47
1:A:733:TYR:CE2	10:A:2147:HOH:O	2.47	0.47
1:A:171[B]:GLU:CG	1:A:341[B]:LYS:HE3	2.42	0.46
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.29	0.46
1:A:303:GLN:NE2	1:A:325:VAL:HG13	2.31	0.46
1:A:412:PRO:HA	1:A:589[B]:ASN:OD1	2.15	0.46
1:A:239[A]:VAL:HG22	1:A:247:ASN:CG	2.41	0.45
1:A:90[B]:PHE:CZ	1:A:94:LYS:HD3	2.52	0.44
1:A:347:HIS:HE1	10:A:2112:HOH:O	1.99	0.44
1:A:589[A]:ASN:OD1	10:A:2417:HOH:O	2.17	0.44
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.00	0.43
1:A:688[A]:ARG:CZ	10:A:1878:HOH:O	2.66	0.43
10:A:2092:HOH:O	3:D:1:NAG:H81	2.18	0.43
1:A:443[B]:GLN:HG3	1:A:444:GLU:CD	2.44	0.43
10:A:2020:HOH:O	3:D:1:NAG:H83	2.18	0.43
1:A:663[A]:MET:HE3	1:A:663[A]:MET:HB2	1.72	0.42
1:A:236:ALA:O	1:A:239[A]:VAL:HG13	2.19	0.42
1:A:132:ASN:HD21	1:A:136:ASN:HD22	1.66	0.42
1:A:347:HIS:CE1	10:A:2112:HOH:O	2.72	0.42
1:A:325:VAL:HB	1:A:326:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HA	1:A:344:MET:O	2.20	0.41
1:A:468:PRO:HG2	1:A:603[A]:VAL:HG21	2.01	0.41
1:A:303:GLN:HE21	1:A:325:VAL:CG1	2.34	0.41
1:A:387:ASP:HA	1:A:388:PRO:HA	1.93	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.88	0.40

All (4) 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)
10:A:1986:HOH:O	10:A:2331:HOH:O[2_565]	1.93	0.27
10:A:2034:HOH:O	10:A:2161:HOH:O[2_565]	1.95	0.25
1:A:656[B]:SER:OG	10:A:2128:HOH:O[4_566]	2.06	0.14
1:A:656[B]:SER:O	10:A:2128:HOH:O[4_566]	2.11	0.09

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	741/709 (104%)	718 (97%)	21 (3%)	2 (0%)	36 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	A	243	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	645/605 (107%)	631 (98%)	14 (2%)	45 15

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	174[A]	LEU
1	A	174[B]	LEU
1	A	189	GLU
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	443[A]	GLN
1	A	443[B]	GLN
1	A	505	GLU
1	A	537	TYR
1	A	542	GLU
1	A	557	GLU
1	A	600	TYR
1	A	719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	97	GLN
1	A	136	ASN
1	A	303	GLN
1	A	618	HIS

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 (i)

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.56	0	17,19,21	1.32	1 (5%)
2	NAG	B	2	2	14,14,15	0.62	0	17,19,21	0.87	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.76	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	1.14	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.94	0	17,19,21	1.44	2 (11%)
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
3	BMA	D	3	3	11,11,12	0.60	0	15,15,17	0.79	0
4	NAG	E	1	1,4	14,14,15	0.84	0	17,19,21	1.33	3 (17%)
4	NAG	E	2	4	14,14,15	0.64	0	17,19,21	1.32	3 (17%)
4	BMA	E	3	4	11,11,12	0.62	0	15,15,17	0.81	1 (6%)
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	1.04	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	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.08	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O5-C1-C2	-3.62	105.69	111.29
3	D	1	NAG	O5-C1-C2	-3.41	106.01	111.29
4	E	1	NAG	O5-C1-C2	-3.25	106.27	111.29
3	D	1	NAG	O5-C5-C4	-3.18	103.10	110.83
3	D	2	NAG	C8-C7-N2	2.69	120.58	116.12
4	E	2	NAG	C8-C7-N2	2.53	120.32	116.12
2	C	1	NAG	O5-C1-C2	-2.47	107.47	111.29
3	D	2	NAG	O7-C7-C8	-2.37	117.83	122.05
4	E	2	NAG	O7-C7-C8	-2.22	118.09	122.05
2	B	2	NAG	C2-N2-C7	2.18	125.83	122.90
4	E	2	NAG	C3-C4-C5	-2.13	106.37	110.23
4	E	3	BMA	O3-C3-C2	-2.12	105.73	110.05
2	C	2	NAG	O7-C7-N2	2.08	125.66	121.98
2	C	2	NAG	O5-C5-C6	2.05	111.66	107.66
4	E	1	NAG	C6-C5-C4	-2.01	108.09	113.02
4	E	1	NAG	O4-C4-C5	-2.01	104.38	109.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

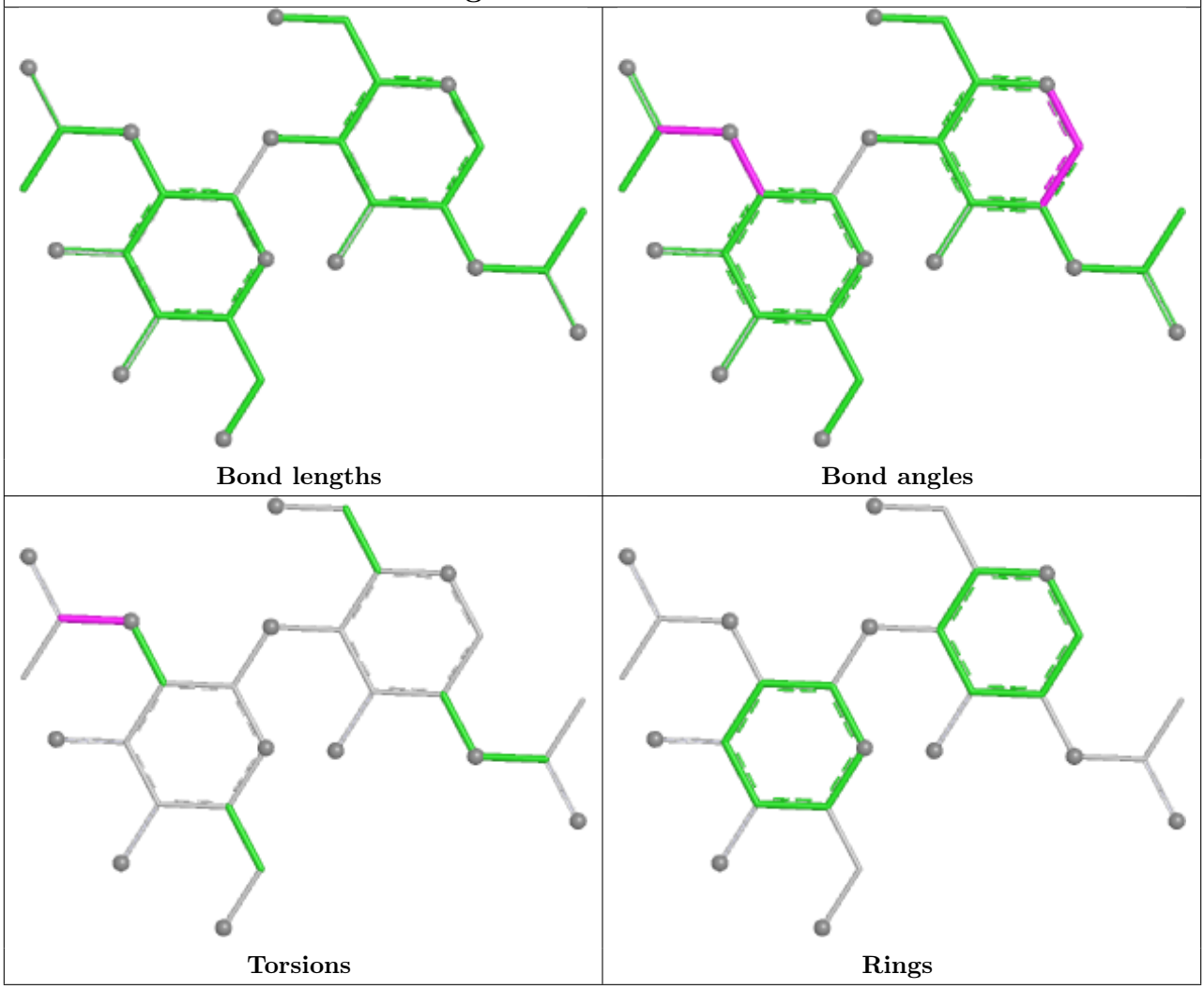
There are no ring outliers.

2 monomers are involved in 3 short contacts:

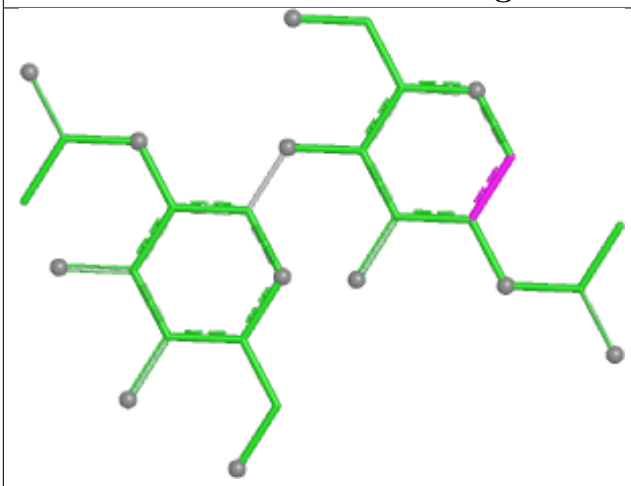
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	2	0
2	B	2	NAG	1	0

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

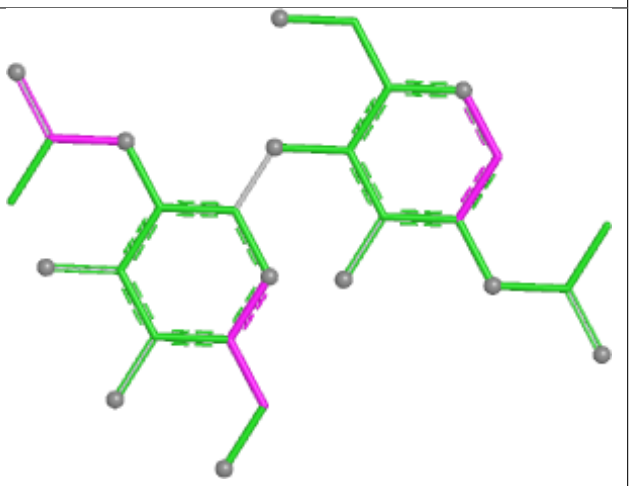
Oligosaccharide Chain B



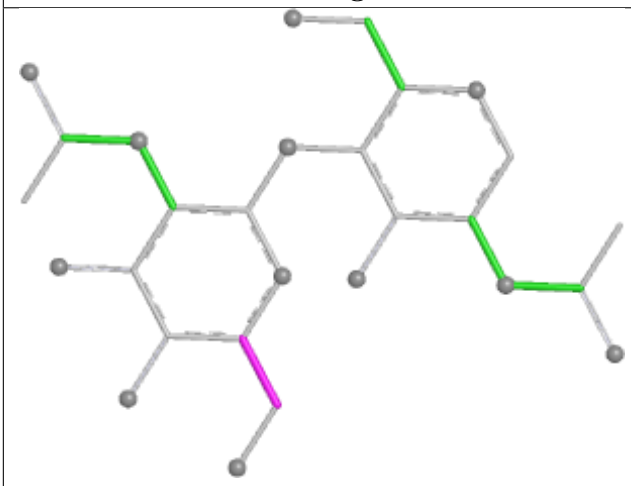
Oligosaccharide Chain C



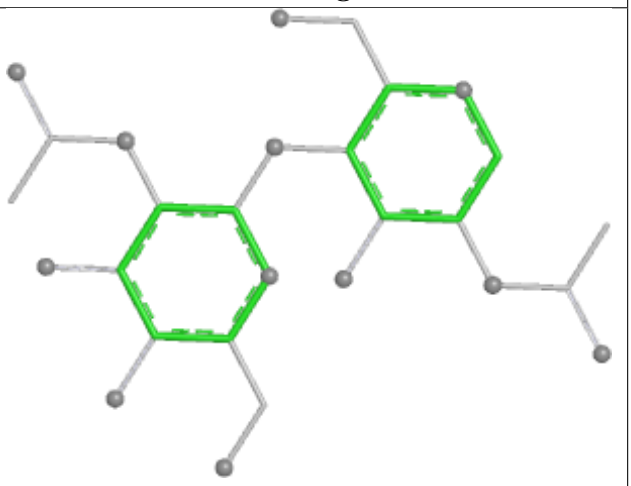
Bond lengths



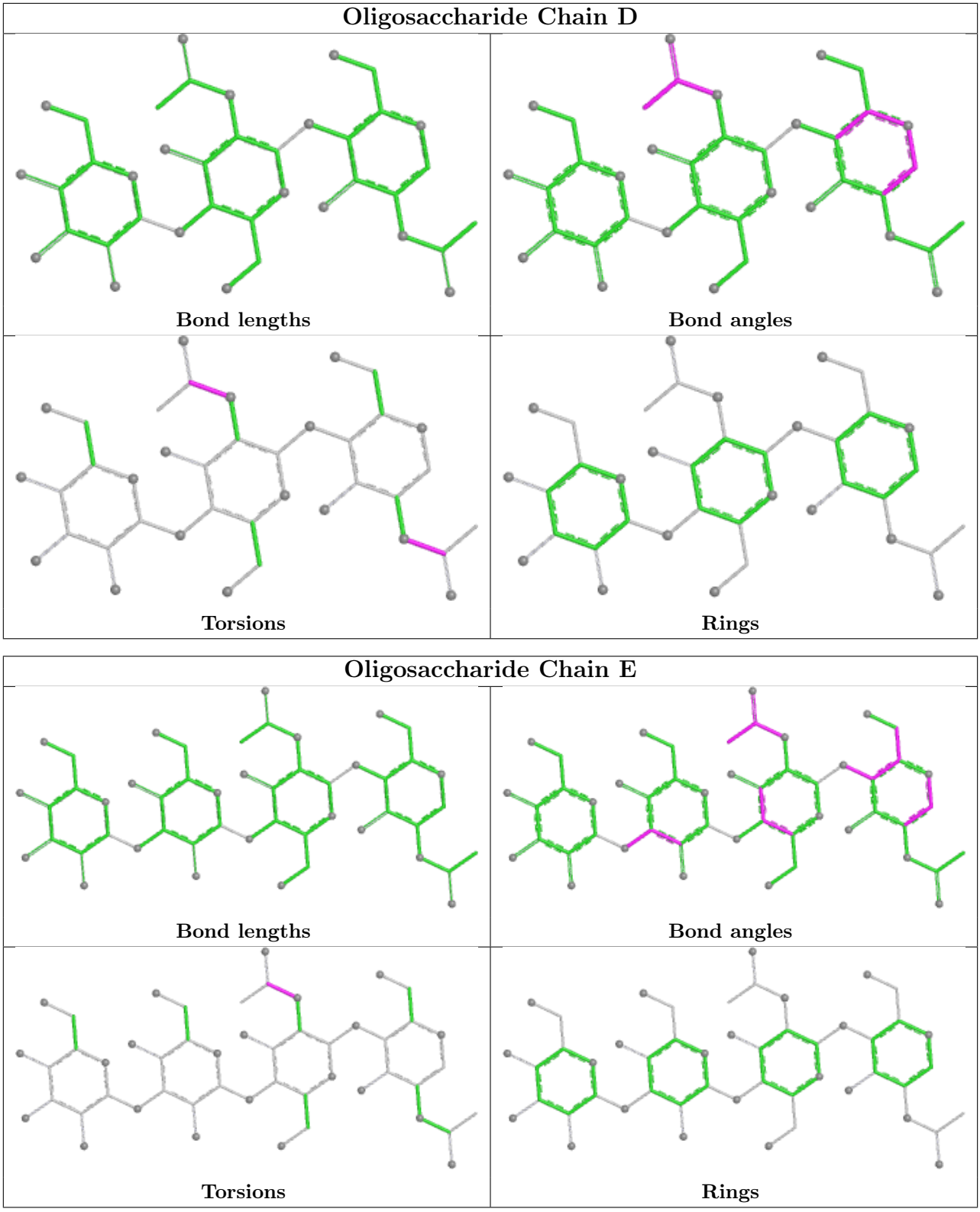
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	YBY	A	1	-	26,26,26	0.97	0	35,35,35	1.76	8 (22%)
5	NAG	A	1759	1	14,14,15	0.50	0	17,19,21	1.26	1 (5%)
5	NAG	A	1757	1	14,14,15	0.62	0	17,19,21	1.28	2 (11%)
5	NAG	A	1760	1	14,14,15	0.63	0	17,19,21	1.57	5 (29%)

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
9	YBY	A	1	-	-	3/25/25/25	0/1/1/1
5	NAG	A	1759	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1757	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1760	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1	YBY	C14-C13-N12	-4.64	101.23	110.83
9	A	1	YBY	C7-C6-N10	-3.39	102.70	110.57
9	A	1	YBY	C19-C17-I18	3.38	123.02	119.76
5	A	1759	NAG	O5-C5-C6	3.28	114.05	107.66
9	A	1	YBY	C5-C6-C7	-3.25	102.64	110.35
5	A	1760	NAG	C1-O5-C5	3.22	116.50	112.19
9	A	1	YBY	O9-C7-C6	3.15	124.17	113.51
9	A	1	YBY	O9-C7-O8	-2.99	117.30	124.08
5	A	1760	NAG	O3-C3-C4	-2.62	104.20	110.38
9	A	1	YBY	O26-C11-N10	-2.35	117.65	122.67
5	A	1760	NAG	O7-C7-C8	-2.33	117.91	122.05
5	A	1760	NAG	C2-N2-C7	-2.21	119.94	122.90
5	A	1757	NAG	C4-C3-C2	2.17	114.20	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1757	NAG	C1-C2-N2	-2.11	107.11	110.43
5	A	1760	NAG	C8-C7-N2	2.06	119.53	116.12
9	A	1	YBY	O26-C11-N12	2.05	127.04	122.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1757	NAG	C8-C7-N2-C2
5	A	1757	NAG	O7-C7-N2-C2
9	A	1	YBY	N12-C13-C14-C15
9	A	1	YBY	C23-C13-C14-C15
9	A	1	YBY	C4-C5-C6-N10

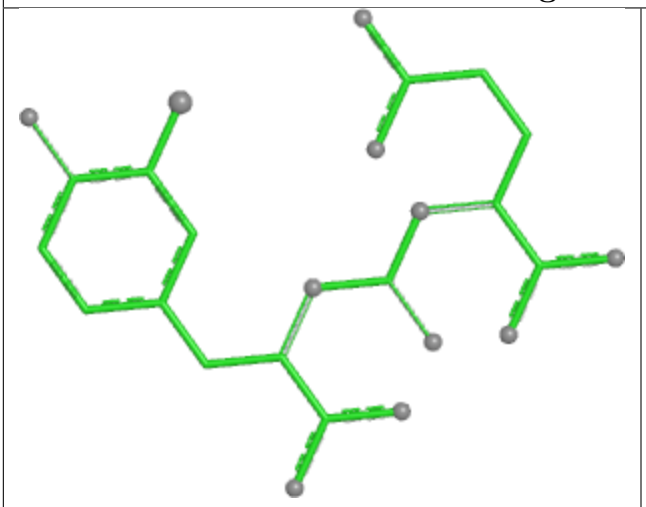
There are no ring outliers.

1 monomer is involved in 1 short contact:

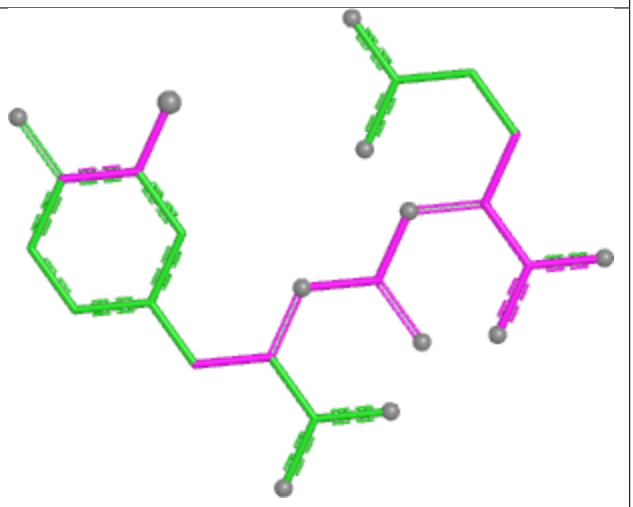
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	NAG	1	0

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

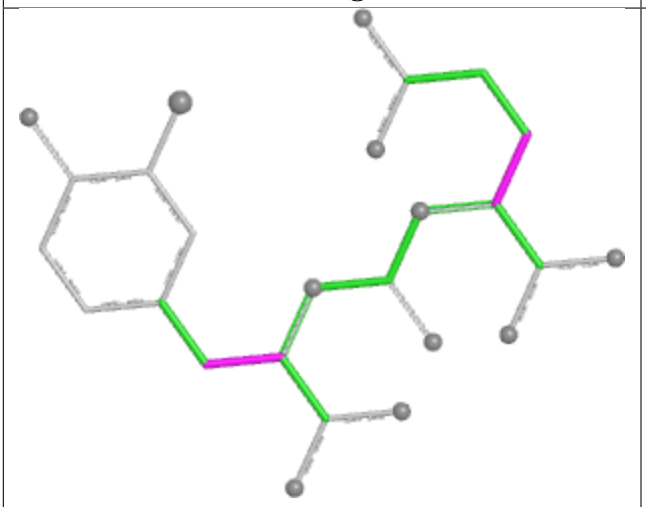
Ligand YBY A 1



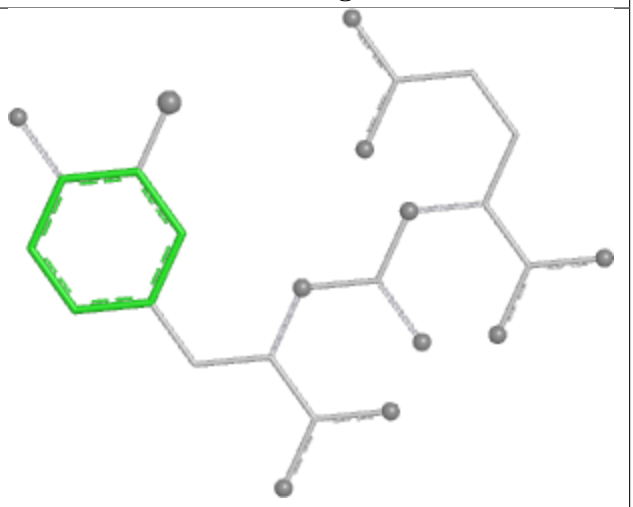
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	691/709 (97%)	-0.05	16 (2%) 61 71	8, 23, 41, 67	57 (8%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	4.4
1	A	544	ASN	3.4
1	A	656[A]	SER	3.3
1	A	506	PHE	2.9
1	A	652	ASP	2.8
1	A	543	THR	2.7
1	A	653	PHE	2.7
1	A	153	ASN	2.7
1	A	486	GLU	2.5
1	A	155[A]	SER	2.3
1	A	152	GLU	2.3
1	A	334	THR	2.2
1	A	131	ILE	2.2
1	A	719	VAL	2.0
1	A	750	ALA	2.0
1	A	507	SER	2.0

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

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

6.3 Carbohydrates

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,

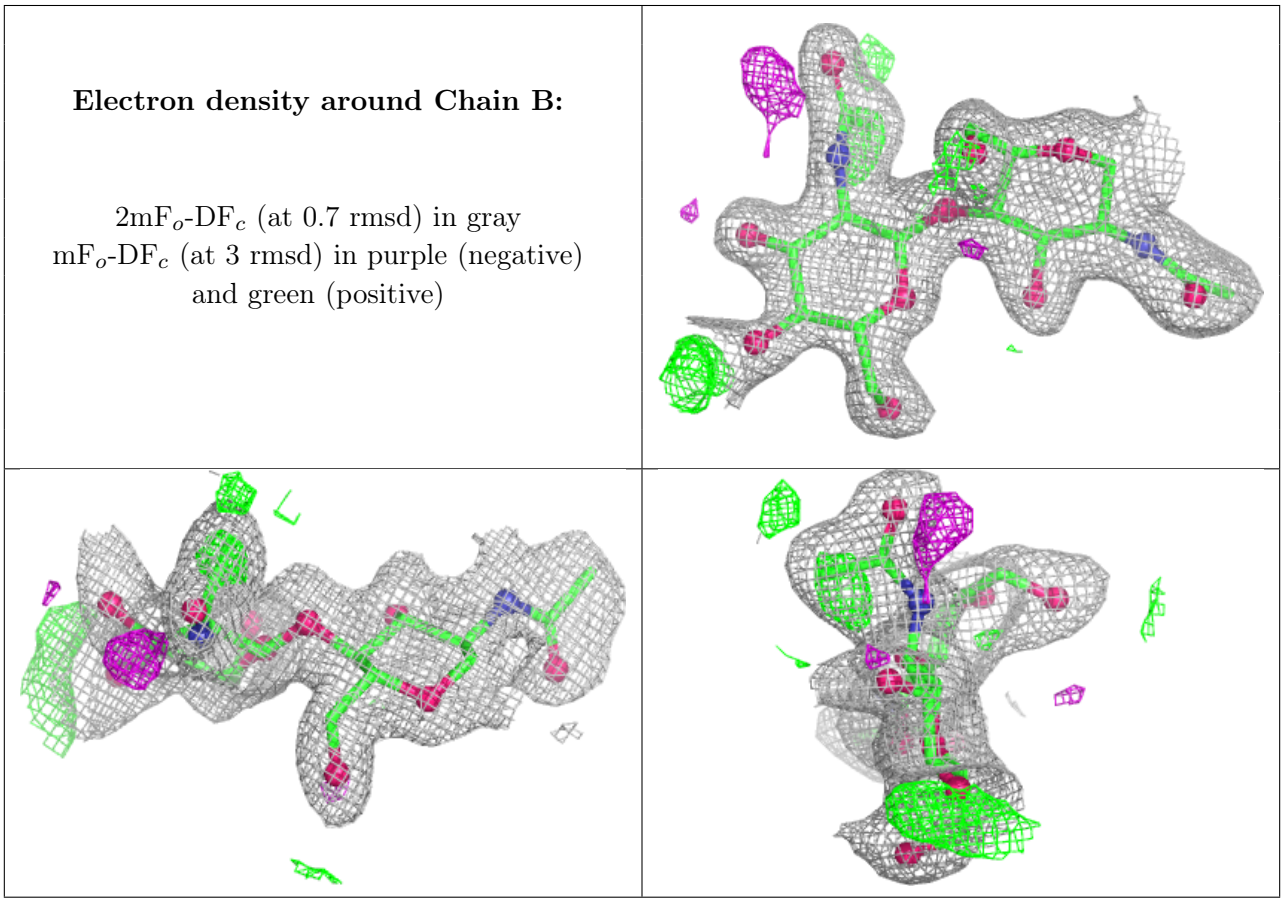
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	D	3	11/12	0.74	0.12	55,57,61,63	0
2	NAG	B	2	14/15	0.75	0.13	43,50,53,56	0
2	NAG	C	2	14/15	0.79	0.12	54,57,62,63	0
3	NAG	D	2	14/15	0.84	0.11	35,42,49,50	0
4	NAG	E	2	14/15	0.86	0.11	33,36,44,47	0
2	NAG	C	1	14/15	0.87	0.10	37,40,43,49	0
4	MAN	E	4	11/12	0.88	0.09	38,41,45,48	0
3	NAG	D	1	14/15	0.90	0.09	27,31,35,39	0
4	BMA	E	3	11/12	0.91	0.07	32,34,36,37	0
2	NAG	B	1	14/15	0.91	0.09	32,39,43,47	0
4	NAG	E	1	14/15	0.94	0.08	21,26,33,43	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.

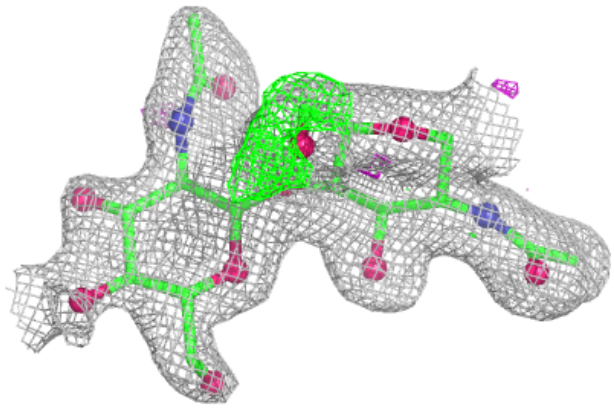
Electron density around Chain B:

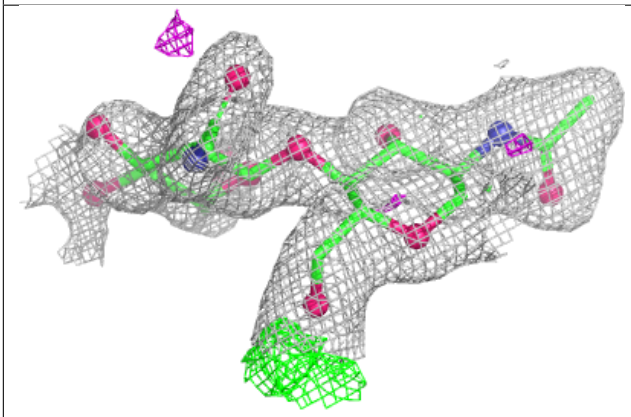
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

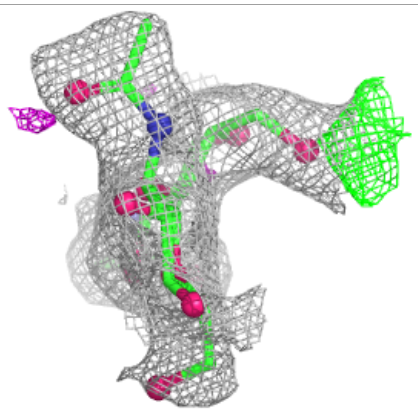


Electron density around Chain C:

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

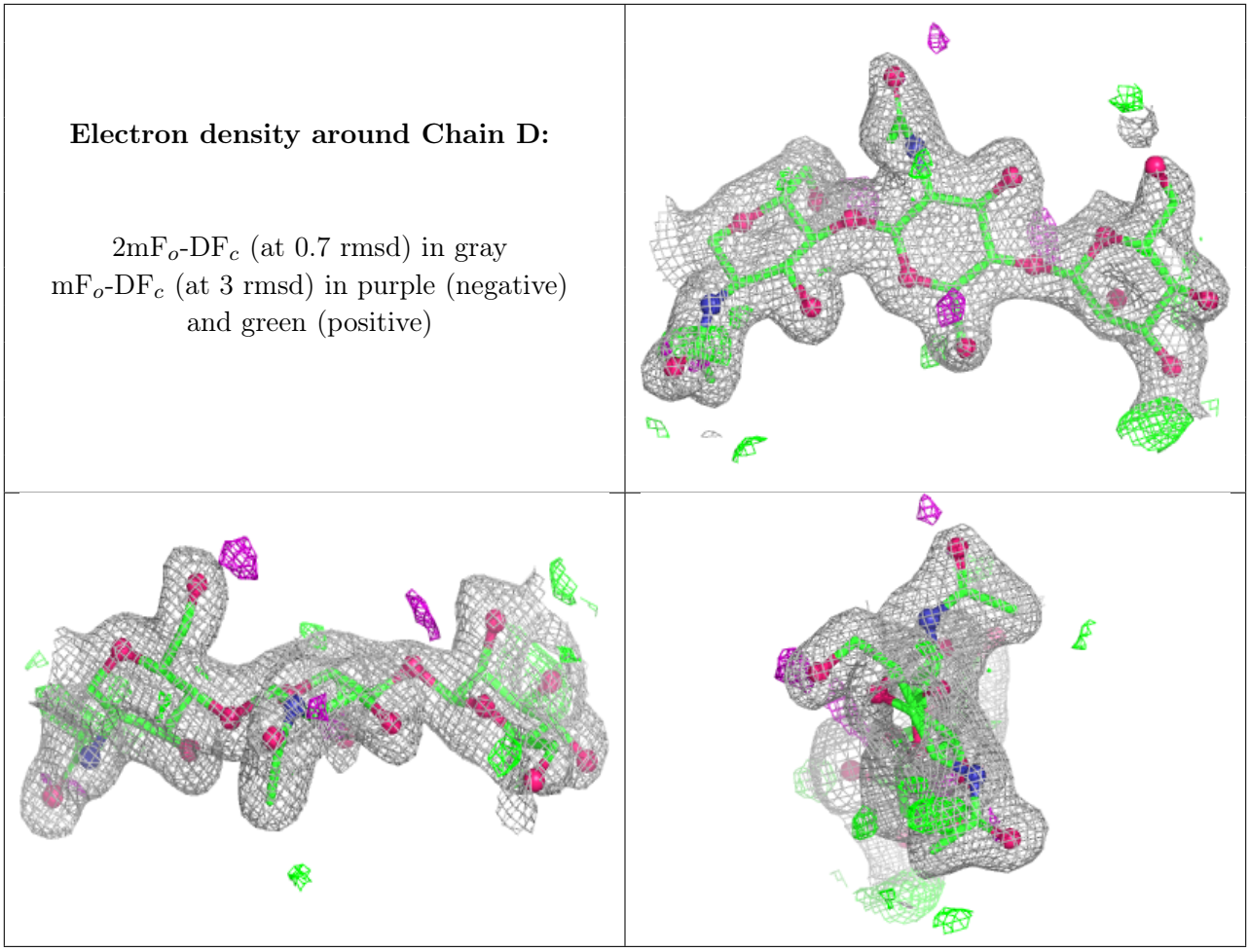






Electron density around Chain D:

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



Electron density around Chain E:

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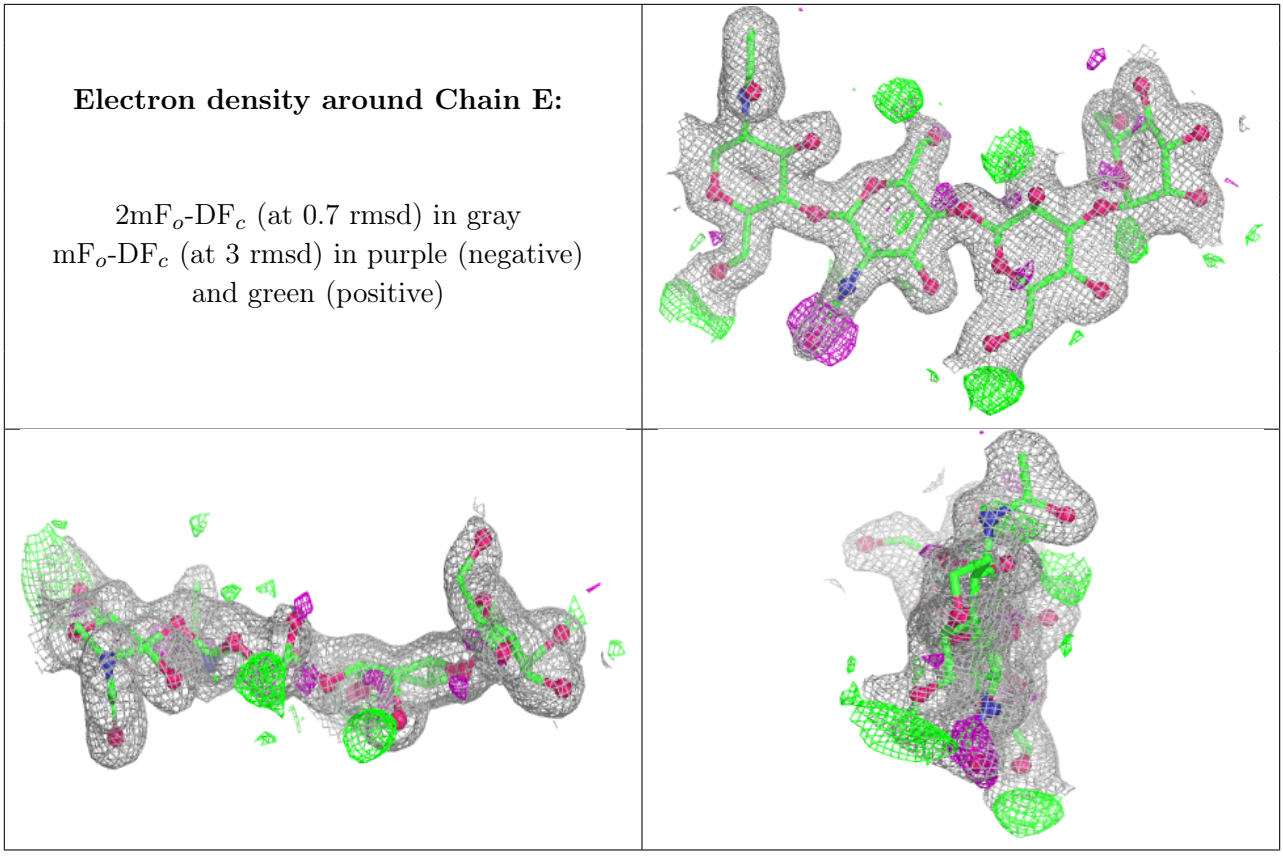
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

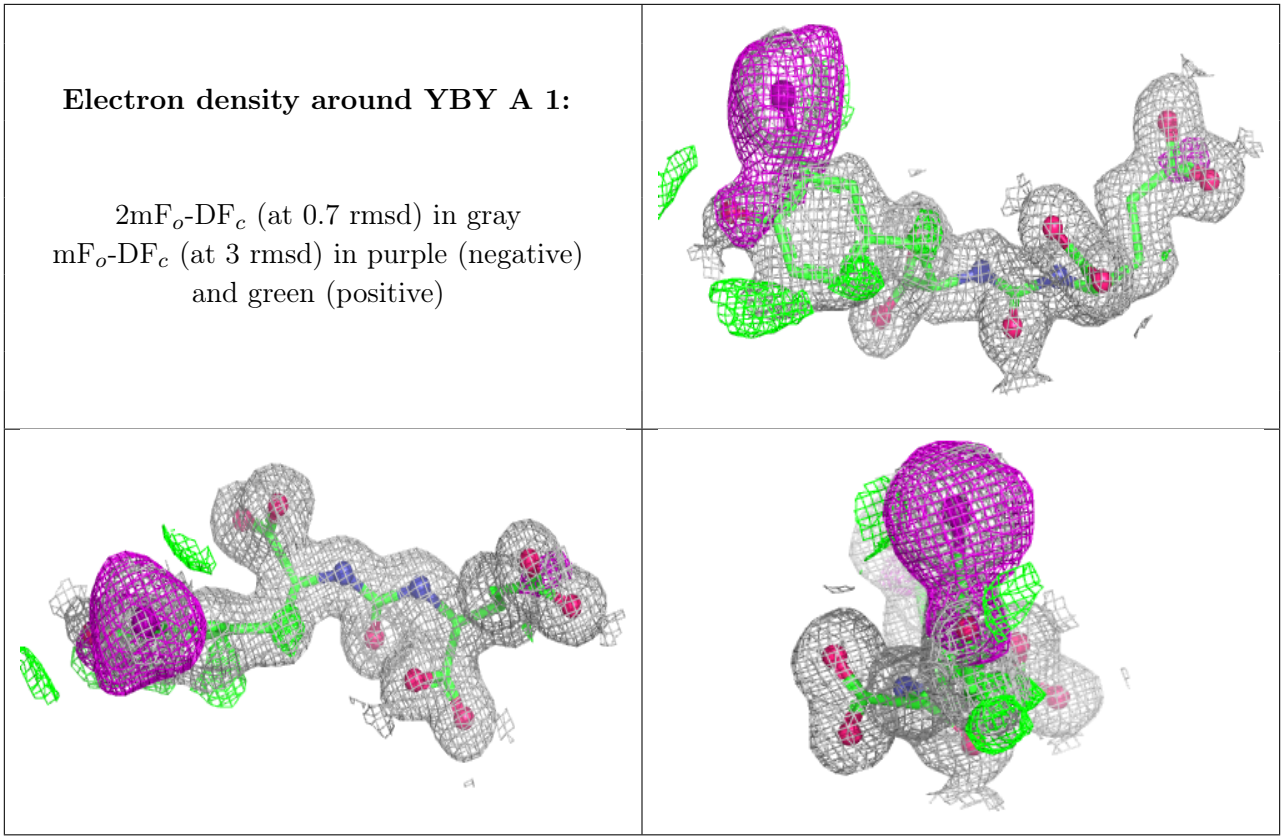
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	A	1757	14/15	0.74	0.15	43,49,53,53	0
5	NAG	A	1759	14/15	0.76	0.13	59,64,67,67	0
5	NAG	A	1760	14/15	0.89	0.10	28,40,46,48	0
9	YBY	A	1	26/26	0.93	0.11	16,20,38,48	0
6	ZN	A	1752	1/1	1.00	0.01	19,19,19,19	0
7	CA	A	1753	1/1	1.00	0.01	15,15,15,15	0
8	CL	A	1754	1/1	1.00	0.04	22,22,22,22	0
6	ZN	A	1751	1/1	1.00	0.01	18,18,18,18	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 YBY A 1:

$2mF_o$-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.