Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:10 AM BST

PDB ID	:	1H1I
Title	:	CRYSTAL STRUCTURE OF QUERCETIN 2,3-DIOXYGENASE ANAEROBICALLY COMPLEXED WITH THE SUBSTRATE QUERCETN
Authors	:	Steiner, R.A.; Dijkstra, B.W.
Deposited on	:	2002-07-15
Resolution	:	1.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

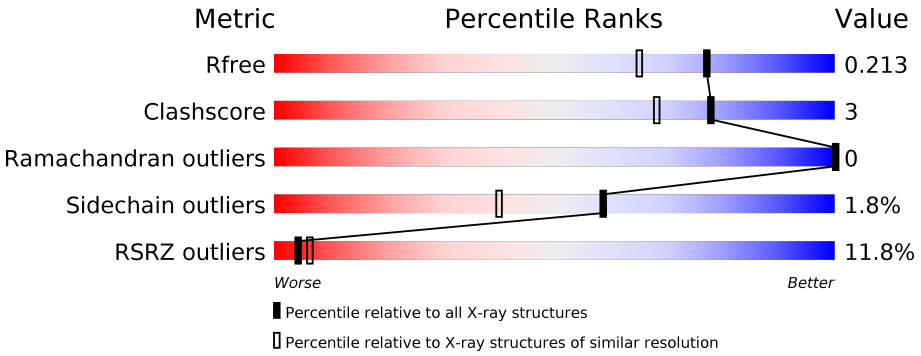
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	350	8% 92% 6%
1	B	350	10% 93% 5%
1	C	350	15% 91% 6%
1	D	350	13% 93% 5%
2	E	2	50% 50%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	100%

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
6	MPD	B	1358	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12575 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.

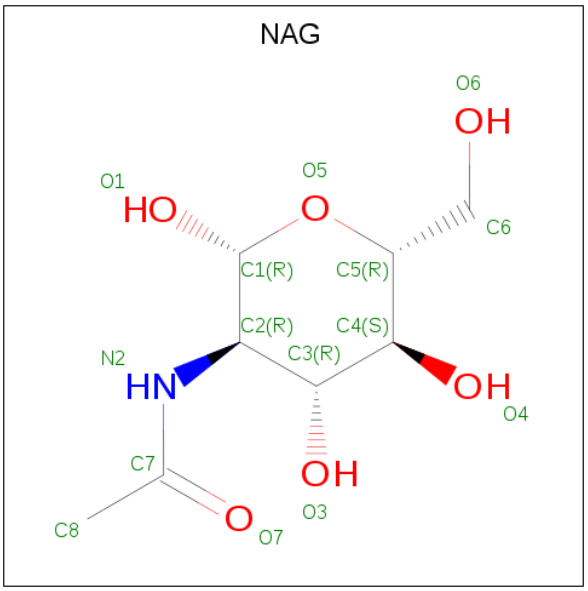
- Molecule 1 is a protein called QUERCETIN 2,3-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	7	0
			2665	1687	433	540	5			
1	B	346	Total	C	N	O	S	0	7	0
			2674	1692	433	543	6			
1	C	343	Total	C	N	O	S	0	2	0
			2642	1676	429	532	5			
1	D	343	Total	C	N	O	S	0	3	0
			2651	1681	431	534	5			

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

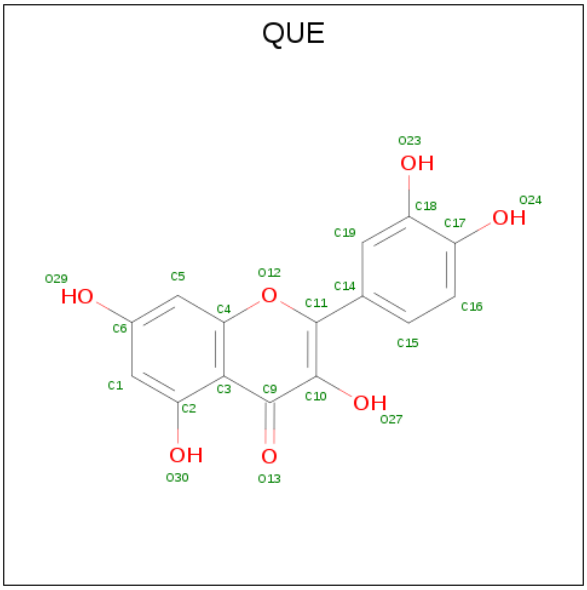


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

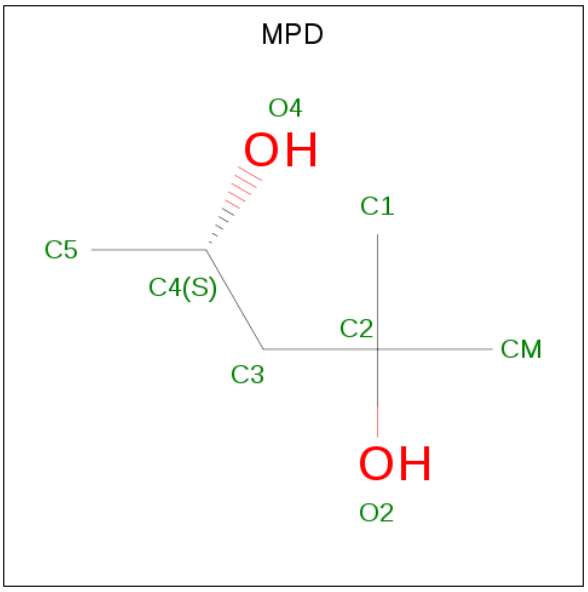
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cu 1 1	0	0
4	A	1	Total Cu 1 1	0	0
4	D	1	Total Cu 1 1	0	0
4	C	1	Total Cu 1 1	0	0

- Molecule 5 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: $C_{15}H_{10}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 22 15 7	0	0
5	B	1	Total C O 22 15 7	0	0
5	C	1	Total C O 22 15 7	0	0
5	D	1	Total C O 22 15 7	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	C	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

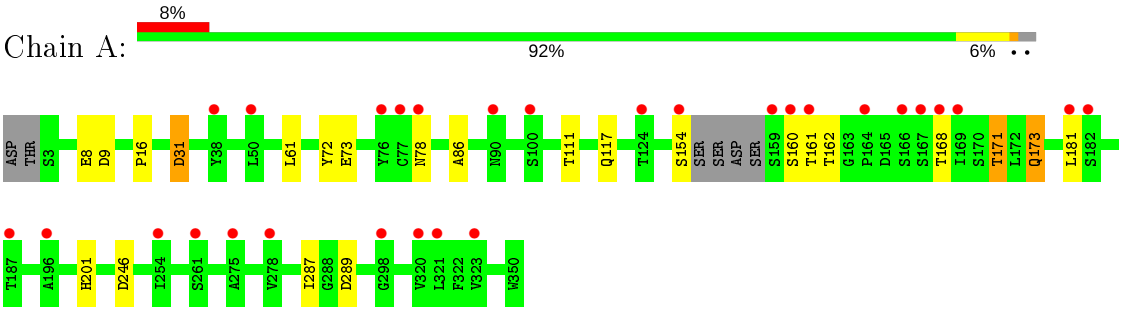
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	427	Total O 427 427	0	0
7	B	378	Total O 378 378	0	0
7	C	370	Total O 370 370	0	0
7	D	364	Total O 364 364	0	0

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.

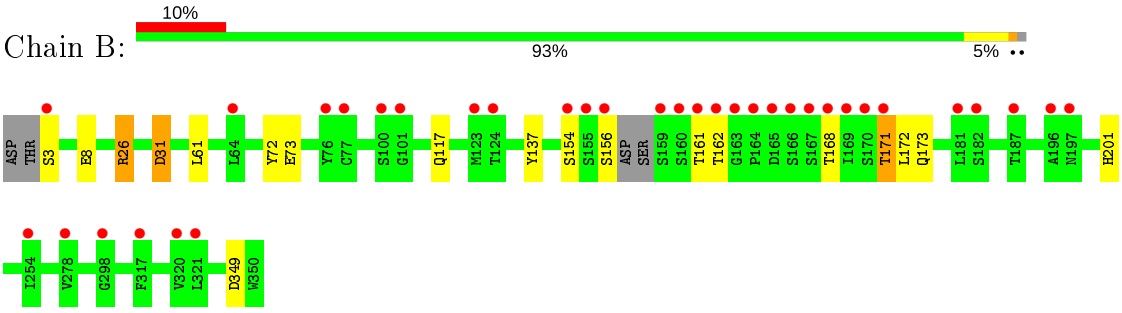
- Molecule 1: QUERCETIN 2,3-DIOXYGENASE

Chain A:



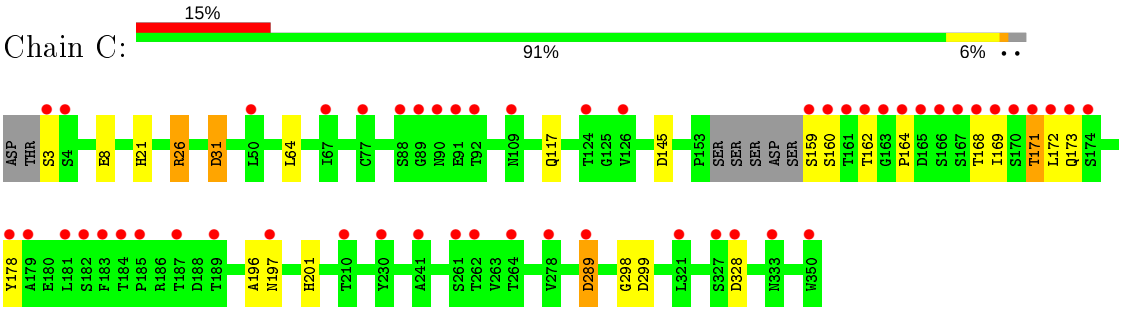
- Molecule 1: QUERCETIN 2,3-DIOXYGENASE

Chain B:



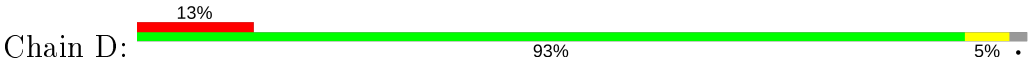
- Molecule 1: QUERCETIN 2,3-DIOXYGENASE

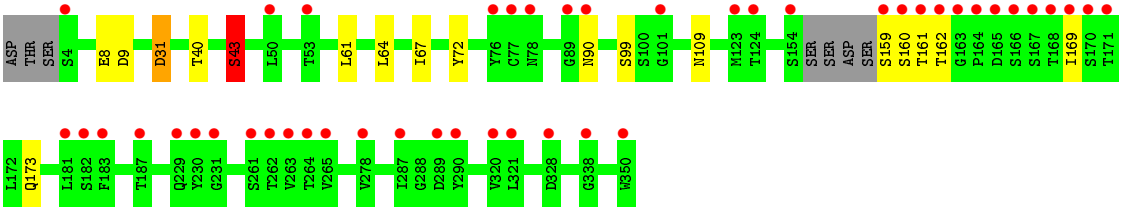
Chain C:



- Molecule 1: QUERCETIN 2,3-DIOXYGENASE

Chain D:





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

Chain E:

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

Chain F:

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

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.30Å 55.74Å 124.16Å 90.00° 98.39° 90.00°	Depositor
Resolution (Å)	49.39 – 1.75 47.02 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.39-1.75) 99.5 (47.02-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.148 , 0.183 0.189 , 0.213	Depositor DCC
R_{free} test set	7473 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12575	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: MPD, QUE, NAG, CU

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	0.84	0/2777	0.86	4/3806 (0.1%)
1	B	0.74	0/2788	0.82	2/3820 (0.1%)
1	C	0.73	0/2732	0.81	5/3746 (0.1%)
1	D	0.74	0/2746	0.80	3/3764 (0.1%)
All	All	0.77	0/11043	0.82	14/15136 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	31	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	31	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	31	ASP	CB-CG-OD2	6.15	123.84	118.30
1	C	289	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	299	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	43	SER	CA-CB-OG	-5.36	96.73	111.20
1	B	349	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	9	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	145	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	9	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	289	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	31	ASP	CB-CG-OD2	5.02	122.82	118.30

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	2665	0	2460	16	0
1	B	2674	0	2475	14	0
1	C	2642	0	2447	16	0
1	D	2651	0	2453	9	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	42	0	39	0	0
3	D	42	0	39	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	22	0	5	2	0
5	B	22	0	5	2	0
5	C	22	0	5	1	0
5	D	22	0	5	0	0
6	A	8	0	14	3	0
6	B	16	0	28	6	0
6	C	8	0	14	3	0
7	A	427	0	0	5	0
7	B	378	0	0	3	0
7	C	370	0	0	5	0
7	D	364	0	0	5	0
All	All	12575	0	10168	62	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 3.

All (62) 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:C:196:ALA:O	1:C:197:ASN:HB3	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1357:MPD:H32	6:B:1358:MPD:H32	1.50	0.93
1:B:8[A]:GLU:HG2	7:B:2003:HOH:O	1.73	0.88
1:D:8[A]:GLU:HG2	7:D:2010:HOH:O	1.74	0.87
1:A:173:GLN:HE21	1:A:173:GLN:H	1.21	0.84
1:A:8[A]:GLU:HG2	7:A:2014:HOH:O	1.78	0.82
6:B:1357:MPD:C3	6:B:1358:MPD:H32	2.11	0.81
1:C:8:GLU:HG2	7:C:2009:HOH:O	1.79	0.81
1:B:201:HIS:CE1	6:B:1358:MPD:HM1	2.26	0.71
1:A:171:THR:HG23	7:A:2215:HOH:O	1.94	0.68
6:A:1359:MPD:H32	6:C:1351:MPD:H32	1.78	0.66
1:A:173:GLN:NE2	1:A:173:GLN:H	1.95	0.64
1:C:197:ASN:O	1:C:197:ASN:ND2	2.30	0.63
1:B:31:ASP:HB2	1:B:162:THR:HG23	1.80	0.63
1:D:8[A]:GLU:CG	7:D:2010:HOH:O	2.41	0.62
1:C:172:LEU:HA	7:C:2202:HOH:O	2.02	0.59
1:D:31:ASP:HB2	1:D:162:THR:HG23	1.85	0.58
1:C:64:LEU:HB2	1:C:169:ILE:HD13	1.85	0.57
1:C:196:ALA:O	1:C:197:ASN:CB	2.34	0.56
1:C:8:GLU:CG	7:C:2009:HOH:O	2.44	0.56
1:B:168:THR:O	1:B:171:THR:HB	2.09	0.53
1:B:171:THR:HG22	1:B:172:LEU:HD23	1.91	0.52
1:D:40:THR:H	1:D:43:SER:HB2	1.75	0.52
6:A:1359:MPD:C3	6:C:1351:MPD:H32	2.39	0.51
1:D:173:GLN:HG3	7:D:2195:HOH:O	2.10	0.51
1:A:31:ASP:HB2	1:A:162:THR:HG23	1.93	0.51
1:A:117:GLN:HG3	7:C:2225:HOH:O	2.11	0.51
1:C:168:THR:O	1:C:171:THR:HB	2.11	0.50
1:B:26:ARG:HD3	1:B:137:TYR:CE1	2.47	0.49
1:C:31:ASP:HB2	1:C:162:THR:HG23	1.95	0.49
1:A:201:HIS:CE1	6:A:1359:MPD:HM1	2.47	0.49
1:C:289:ASP:CG	1:C:289:ASP:O	2.51	0.48
1:B:117:GLN:HG3	7:D:2220:HOH:O	2.12	0.48
1:C:173:GLN:HG2	1:C:178:TYR:CE2	2.48	0.48
1:C:201:HIS:CE1	6:C:1351:MPD:HM1	2.48	0.48
1:C:164:PRO:HG2	1:C:169:ILE:HD12	1.96	0.47
5:A:1358:QUE:O27	5:A:1358:QUE:H19	2.15	0.46
1:B:73:GLU:CD	5:B:1356:QUE:H19	2.35	0.46
1:B:8[A]:GLU:CG	7:B:2003:HOH:O	2.45	0.46
1:A:78[B]:ASN:ND2	7:A:2110:HOH:O	2.34	0.46
1:C:26:ARG:HD2	7:C:2053:HOH:O	2.16	0.46
6:B:1357:MPD:H31	6:B:1358:MPD:H32	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:SER:HB2	7:B:2170:HOH:O	2.17	0.45
1:B:61:LEU:HB2	1:B:161:THR:HG23	1.99	0.45
6:B:1358:MPD:H11	1:D:99:SER:HB3	1.99	0.44
1:A:61:LEU:HB2	1:A:161:THR:HG23	2.00	0.43
1:A:168:THR:O	1:A:171:THR:HB	2.19	0.43
1:A:8[A]:GLU:CG	7:A:2014:HOH:O	2.51	0.43
6:B:1357:MPD:H4	6:B:1358:MPD:H13	2.01	0.43
5:C:1358:QUE:O27	5:C:1358:QUE:H19	2.20	0.42
1:B:73:GLU:OE2	5:B:1356:QUE:H19	2.19	0.42
1:A:16:PRO:HB3	1:A:287:ILE:HG21	2.01	0.42
1:C:21:HIS:CG	1:C:298:GLY:HA3	2.55	0.42
1:A:73:GLU:OE2	5:A:1358:QUE:H19	2.20	0.41
1:D:64:LEU:HB2	1:D:169:ILE:HD13	2.02	0.41
1:A:201:HIS:HB3	1:C:117:GLN:NE2	2.36	0.41
1:D:61:LEU:HB2	1:D:161:THR:HG23	2.02	0.41
1:A:86:ALA:HA	1:A:111:THR:O	2.21	0.40
1:A:154:SER:HB2	7:A:2202:HOH:O	2.20	0.40
1:D:109:ASN:HB3	7:D:2133:HOH:O	2.21	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	347/350 (99%)	340 (98%)	7 (2%)	0	100	100
1	B	349/350 (100%)	340 (97%)	9 (3%)	0	100	100
1	C	341/350 (97%)	329 (96%)	12 (4%)	0	100	100
1	D	342/350 (98%)	332 (97%)	10 (3%)	0	100	100
All	All	1379/1400 (98%)	1341 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	295/294 (100%)	290 (98%)	5 (2%)	60	42
1	B	297/294 (101%)	292 (98%)	5 (2%)	60	42
1	C	289/294 (98%)	284 (98%)	5 (2%)	60	42
1	D	290/294 (99%)	284 (98%)	6 (2%)	53	31
All	All	1171/1176 (100%)	1150 (98%)	21 (2%)	59	40

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	TYR
1	A	160	SER
1	A	171	THR
1	A	173	GLN
1	A	181	LEU
1	B	3	SER
1	B	26	ARG
1	B	72	TYR
1	B	156	SER
1	B	171	THR
1	C	3	SER
1	C	26	ARG
1	C	159	SER
1	C	160	SER
1	C	171	THR
1	D	43	SER
1	D	67	ILE
1	D	72	TYR
1	D	90	ASN
1	D	159	SER
1	D	160	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	173	GLN
1	A	245	GLN
1	B	83	GLN
1	C	197	ASN
1	D	90	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

6 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	E	1	1,2	14,14,15	0.55	0	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	1.17	2 (11%)
2	NAG	F	2	2	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
2	NAG	G	2	2	14,14,15	0.56	0	17,19,21	1.22	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	O7-C7-N2	2.75	127.01	121.95
2	F	2	NAG	O7-C7-N2	2.71	126.94	121.95
2	F	1	NAG	O4-C4-C5	-2.61	102.81	109.30
2	F	2	NAG	O7-C7-C8	-2.58	117.27	122.06
2	F	1	NAG	O5-C5-C6	2.40	110.96	107.20
2	E	2	NAG	O4-C4-C5	2.28	114.97	109.30
2	G	2	NAG	C1-O5-C5	2.21	115.19	112.19
2	G	1	NAG	O4-C4-C5	-2.10	104.08	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

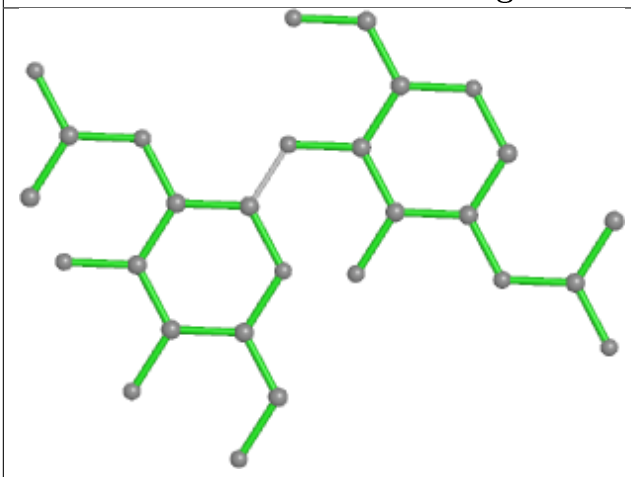
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

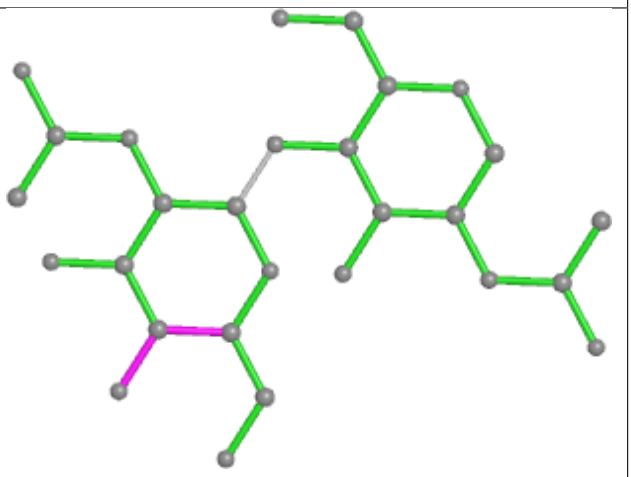
No monomer is involved in short contacts.

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

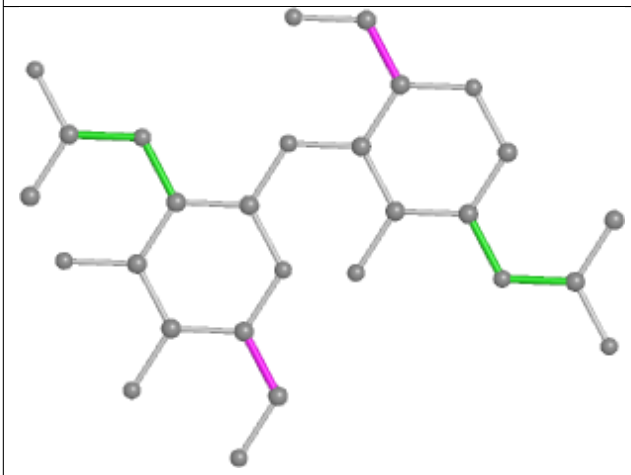
Oligosaccharide Chain E



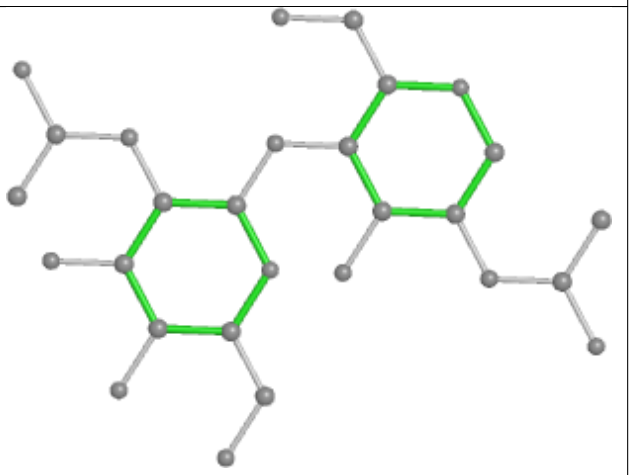
Bond lengths



Bond angles

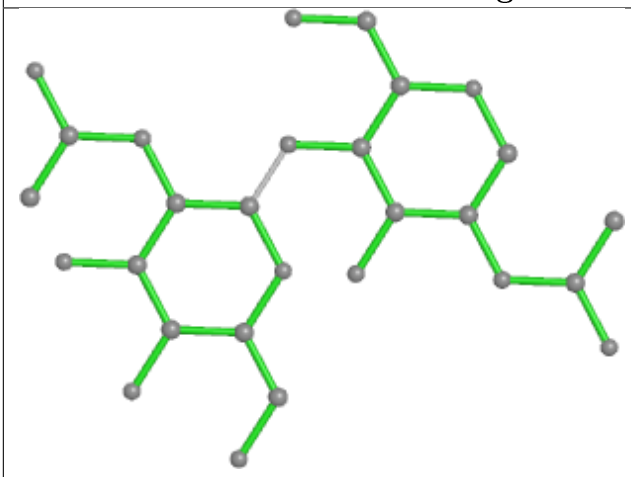


Torsions

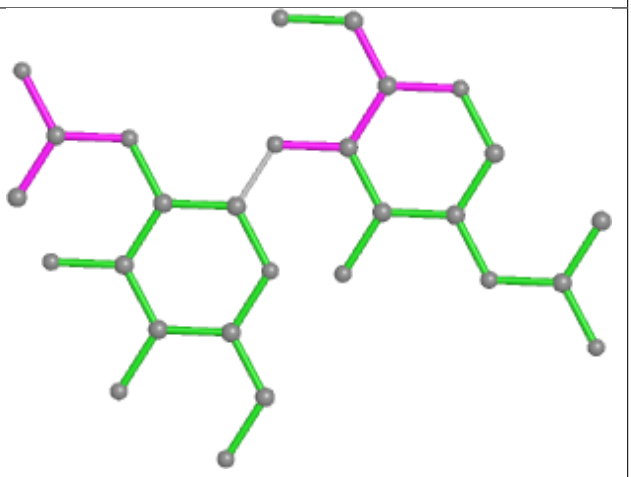


Rings

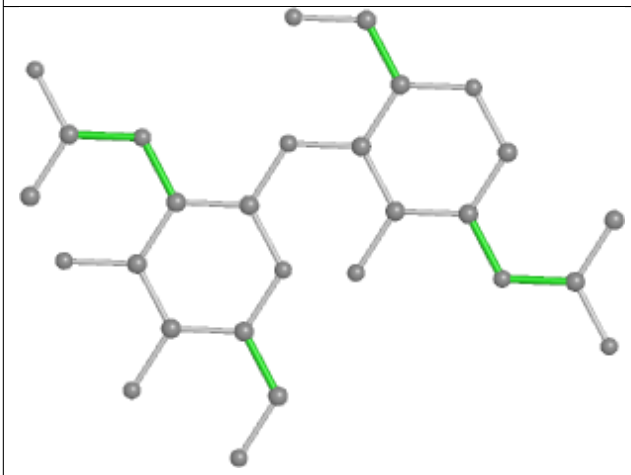
Oligosaccharide Chain F



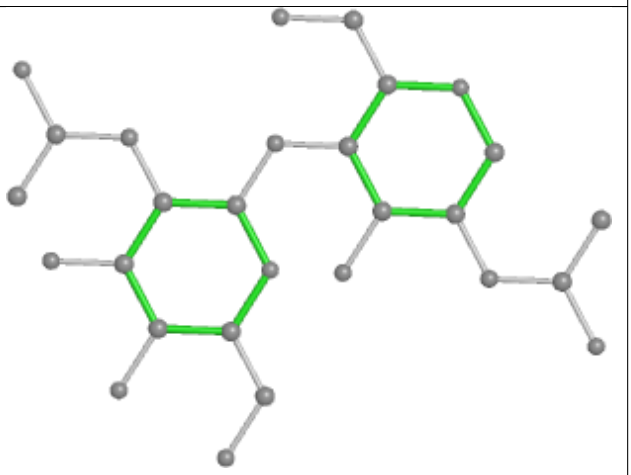
Bond lengths



Bond angles

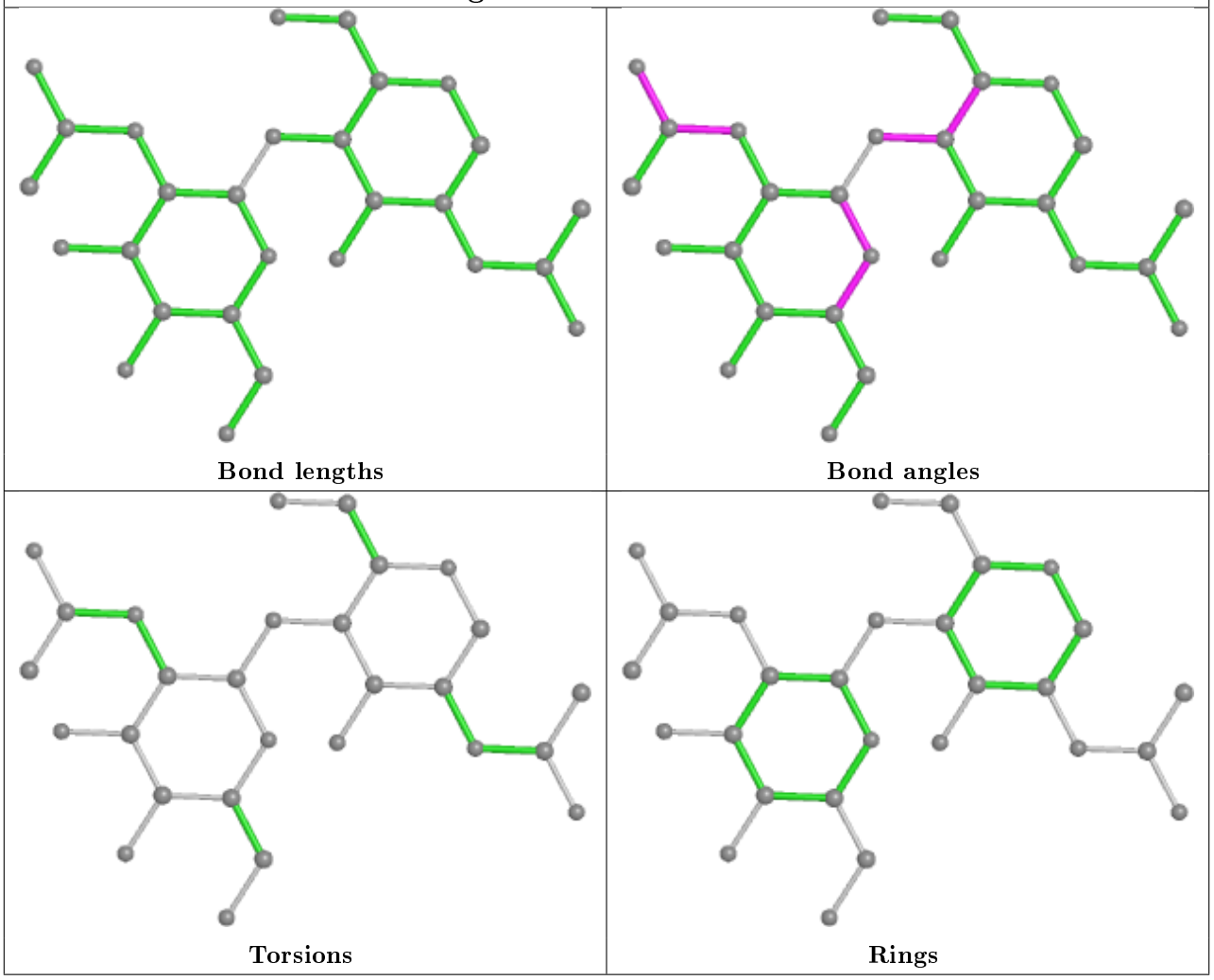


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
3	NAG	D	1354	1	14,14,15	0.83	1 (7%)	17,19,21	1.54	2 (11%)
6	MPD	A	1359	-	7,7,7	0.48	0	9,10,10	1.90	2 (22%)
6	MPD	B	1357	-	7,7,7	0.50	0	9,10,10	2.02	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MPD	C	1351	-	7,7,7	0.45	0	9,10,10	2.09	2 (22%)
3	NAG	C	1355	1	14,14,15	0.70	1 (7%)	17,19,21	1.01	2 (11%)
3	NAG	C	1356	1	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
5	QUE	D	1357	4	21,24,24	2.16	5 (23%)	28,36,36	1.89	8 (28%)
5	QUE	B	1356	4	21,24,24	1.98	3 (14%)	28,36,36	1.66	6 (21%)
3	NAG	A	1354	1	14,14,15	0.73	1 (7%)	17,19,21	1.02	0
3	NAG	B	1351	1	14,14,15	0.58	0	17,19,21	0.79	0
3	NAG	C	1352	1	14,14,15	0.39	0	17,19,21	1.21	1 (5%)
3	NAG	A	1356	1	14,14,15	0.85	0	17,19,21	1.55	1 (5%)
3	NAG	D	1355	1	14,14,15	0.75	0	17,19,21	1.46	2 (11%)
3	NAG	A	1351	1	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
3	NAG	B	1354	1	14,14,15	0.65	0	17,19,21	1.01	1 (5%)
3	NAG	B	1352	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
3	NAG	B	1353	1	14,14,15	0.72	0	17,19,21	1.27	2 (11%)
5	QUE	C	1358	4	21,24,24	1.89	3 (14%)	28,36,36	1.82	7 (25%)
6	MPD	B	1358	-	7,7,7	0.41	0	9,10,10	1.67	2 (22%)
3	NAG	D	1351	1	14,14,15	0.44	0	17,19,21	1.20	2 (11%)
3	NAG	A	1355	1	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
5	QUE	A	1358	4	21,24,24	2.09	6 (28%)	28,36,36	1.67	6 (21%)

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
3	NAG	D	1354	1	-	1/6/23/26	0/1/1/1
6	MPD	A	1359	-	-	1/5/5/5	-
6	MPD	B	1357	-	-	2/5/5/5	-
6	MPD	C	1351	-	-	2/5/5/5	-
3	NAG	C	1355	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1356	1	-	0/6/23/26	0/1/1/1
5	QUE	D	1357	4	-	2/4/4/4	0/3/3/3
5	QUE	B	1356	4	-	2/4/4/4	0/3/3/3
3	NAG	A	1354	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1351	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1352	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1356	1	-	1/6/23/26	0/1/1/1
3	NAG	D	1355	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1351	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1354	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1352	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
5	QUE	C	1358	4	-	2/4/4/4	0/3/3/3
6	MPD	B	1358	-	-	4/5/5/5	-
3	NAG	D	1351	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
5	QUE	A	1358	4	-	2/4/4/4	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1357	QUE	C18-C17	6.61	1.50	1.40
5	A	1358	QUE	C18-C17	5.39	1.48	1.40
5	C	1358	QUE	C3-C4	5.19	1.48	1.41
5	B	1356	QUE	C3-C4	4.80	1.47	1.41
5	B	1356	QUE	C18-C17	4.80	1.47	1.40
5	A	1358	QUE	C3-C4	4.76	1.47	1.41
5	C	1358	QUE	C18-C17	4.65	1.47	1.40
5	D	1357	QUE	C3-C4	4.64	1.47	1.41
5	A	1358	QUE	C2-C3	3.33	1.49	1.43
5	B	1356	QUE	C14-C11	3.28	1.51	1.46
5	D	1357	QUE	C2-C3	2.93	1.48	1.43
5	A	1358	QUE	C14-C11	2.39	1.50	1.46
5	D	1357	QUE	C14-C11	2.26	1.50	1.46
5	C	1358	QUE	C14-C11	2.24	1.50	1.46
5	A	1358	QUE	C5-C6	2.22	1.41	1.37
3	C	1355	NAG	C1-C2	2.15	1.55	1.52
5	D	1357	QUE	C5-C6	2.13	1.41	1.37
3	D	1354	NAG	C1-C2	2.12	1.55	1.52
3	A	1354	NAG	C1-C2	2.10	1.55	1.52
5	A	1358	QUE	O29-C6	-2.09	1.32	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1351	MPD	CM-C2-C1	-5.30	99.52	110.57
5	D	1357	QUE	O12-C4-C5	5.22	122.22	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1358	QUE	O12-C4-C5	5.14	122.13	116.11
3	A	1356	NAG	C1-O5-C5	5.12	119.14	112.19
6	B	1357	MPD	CM-C2-C1	-5.02	100.12	110.57
5	C	1358	QUE	O12-C4-C5	4.64	121.54	116.11
6	A	1359	MPD	CM-C2-C1	-4.47	101.25	110.57
3	D	1354	NAG	O5-C1-C2	-4.21	104.63	111.29
3	D	1355	NAG	O5-C1-C2	-4.06	104.88	111.29
5	B	1356	QUE	O12-C4-C5	3.97	120.76	116.11
5	C	1358	QUE	C15-C14-C11	-3.82	114.97	120.29
3	D	1354	NAG	C1-O5-C5	3.73	117.25	112.19
3	B	1352	NAG	C1-O5-C5	3.71	117.22	112.19
6	B	1358	MPD	CM-C2-C1	-3.60	103.07	110.57
5	B	1356	QUE	C15-C14-C11	-3.54	115.35	120.29
5	B	1356	QUE	C19-C14-C11	3.54	125.22	120.29
5	A	1358	QUE	C5-C4-C3	-3.39	119.30	123.05
5	D	1357	QUE	C5-C4-C3	-3.35	119.33	123.05
3	B	1353	NAG	O5-C1-C2	-3.16	106.29	111.29
3	C	1352	NAG	C2-N2-C7	3.14	127.38	122.90
5	D	1357	QUE	C15-C14-C11	-3.13	115.92	120.29
5	C	1358	QUE	C10-C9-C3	-3.07	117.09	121.38
5	D	1357	QUE	C14-C19-C18	-2.97	118.32	120.68
5	B	1356	QUE	O12-C4-C3	-2.95	118.13	121.03
5	D	1357	QUE	C10-C9-C3	-2.88	117.35	121.38
3	B	1354	NAG	C1-O5-C5	-2.87	108.30	112.19
5	C	1358	QUE	C19-C14-C11	2.86	124.28	120.29
3	D	1355	NAG	O5-C5-C4	-2.84	103.92	110.83
5	C	1358	QUE	O12-C4-C3	-2.74	118.33	121.03
3	C	1356	NAG	O4-C4-C3	-2.71	104.08	110.35
6	C	1351	MPD	O2-C2-CM	2.68	116.68	108.08
5	C	1358	QUE	C5-C4-C3	-2.64	120.12	123.05
5	D	1357	QUE	O12-C4-C3	-2.63	118.44	121.03
5	A	1358	QUE	C5-C6-C1	2.61	123.05	120.94
5	C	1358	QUE	C5-C6-C1	2.56	123.01	120.94
3	C	1355	NAG	O5-C1-C2	-2.51	107.32	111.29
5	A	1358	QUE	O12-C4-C3	-2.50	118.57	121.03
5	D	1357	QUE	C19-C14-C11	2.44	123.70	120.29
6	A	1359	MPD	O2-C2-CM	2.42	115.84	108.08
5	D	1357	QUE	C5-C6-C1	2.38	122.86	120.94
3	B	1353	NAG	O5-C5-C6	2.37	110.92	107.20
5	A	1358	QUE	C15-C16-C17	-2.37	118.07	120.50
6	B	1358	MPD	C5-C4-C3	2.33	122.67	111.69
5	B	1356	QUE	C10-C9-C3	-2.25	118.23	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1351	NAG	O7-C7-C8	-2.20	117.96	122.06
5	B	1356	QUE	O23-C18-C19	2.20	125.36	119.46
3	A	1351	NAG	O7-C7-C8	-2.16	118.05	122.06
3	C	1355	NAG	C2-N2-C7	-2.14	119.86	122.90
3	D	1351	NAG	C1-O5-C5	2.13	115.08	112.19
3	A	1355	NAG	O7-C7-C8	-2.03	118.29	122.06
6	B	1357	MPD	O2-C2-C1	-2.01	101.63	108.08
5	A	1358	QUE	C15-C14-C11	-2.00	117.50	120.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1357	QUE	C10-C11-C14-C15
5	D	1357	QUE	C10-C11-C14-C19
5	B	1356	QUE	C10-C11-C14-C15
5	B	1356	QUE	C10-C11-C14-C19
5	C	1358	QUE	C10-C11-C14-C15
5	C	1358	QUE	C10-C11-C14-C19
6	B	1358	MPD	C2-C3-C4-C5
5	A	1358	QUE	C10-C11-C14-C15
5	A	1358	QUE	C10-C11-C14-C19
3	D	1354	NAG	C3-C2-N2-C7
3	D	1351	NAG	O5-C5-C6-O6
6	C	1351	MPD	O2-C2-C3-C4
6	B	1357	MPD	C2-C3-C4-C5
6	B	1357	MPD	CM-C2-C3-C4
6	B	1358	MPD	CM-C2-C3-C4
3	A	1356	NAG	C3-C2-N2-C7
6	B	1358	MPD	O2-C2-C3-C4
6	C	1351	MPD	C2-C3-C4-C5
6	A	1359	MPD	C2-C3-C4-C5
3	D	1351	NAG	O7-C7-N2-C2
6	B	1358	MPD	C2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1359	MPD	3	0
6	B	1357	MPD	4	0

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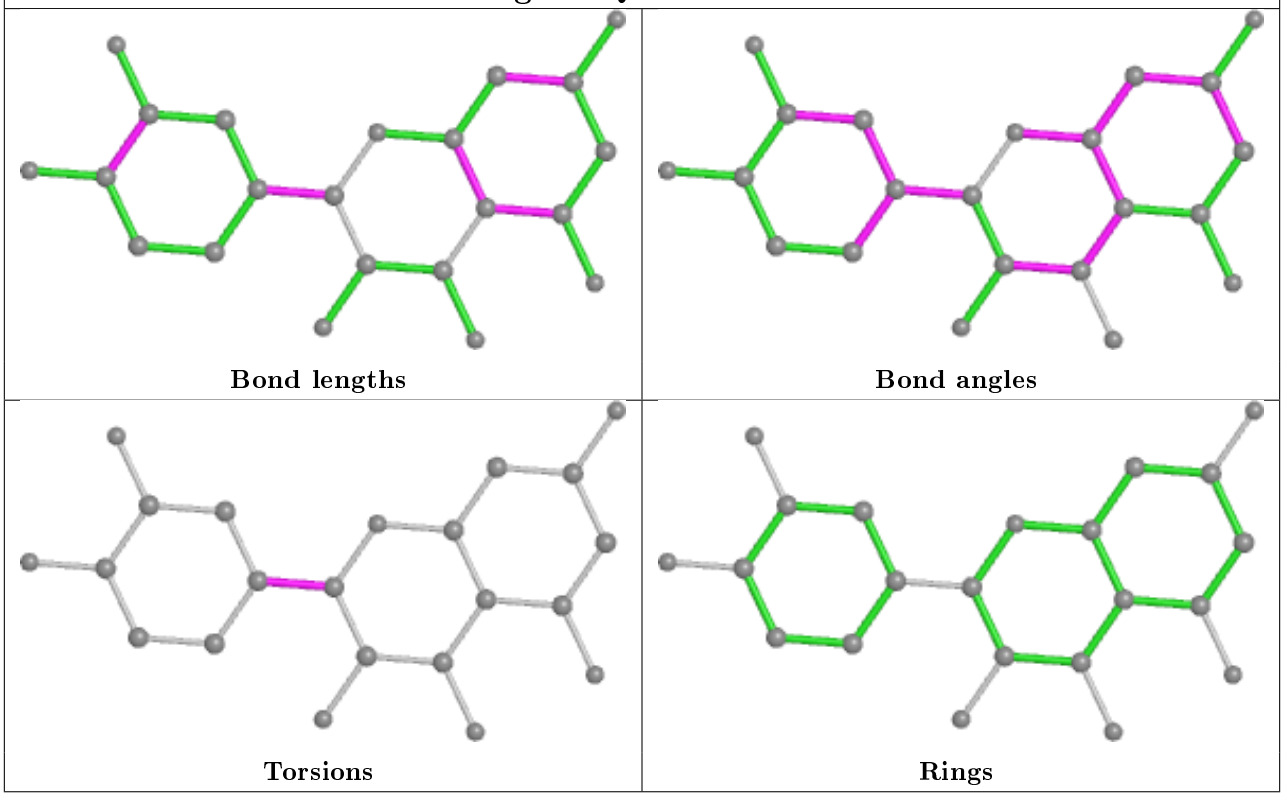
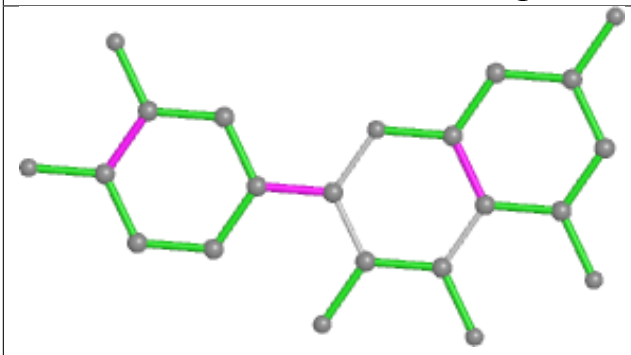
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1351	MPD	3	0
5	B	1356	QUE	2	0
5	C	1358	QUE	1	0
6	B	1358	MPD	6	0
5	A	1358	QUE	2	0

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

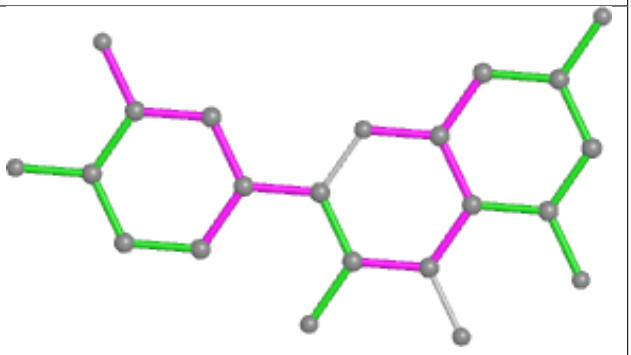
Ligand QUE D 1357



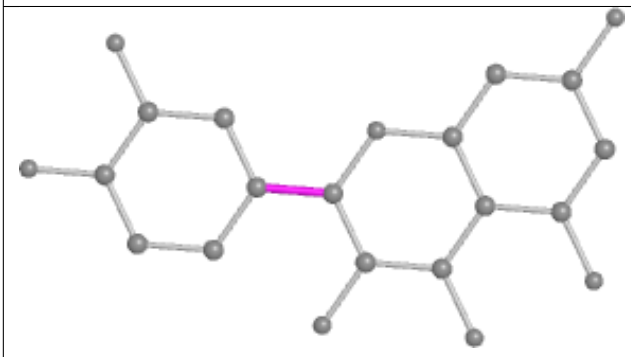
Ligand QUE B 1356



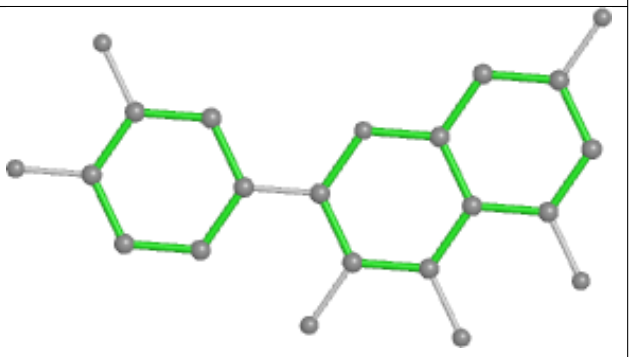
Bond lengths



Bond angles

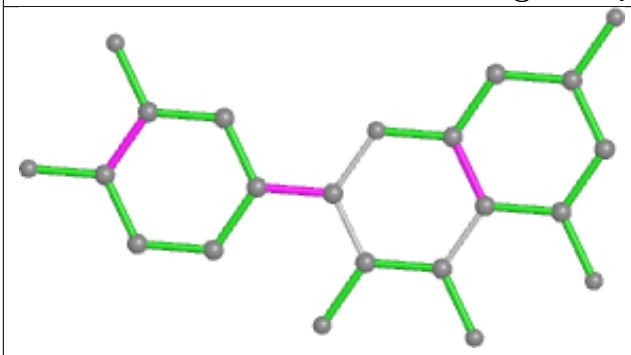


Torsions

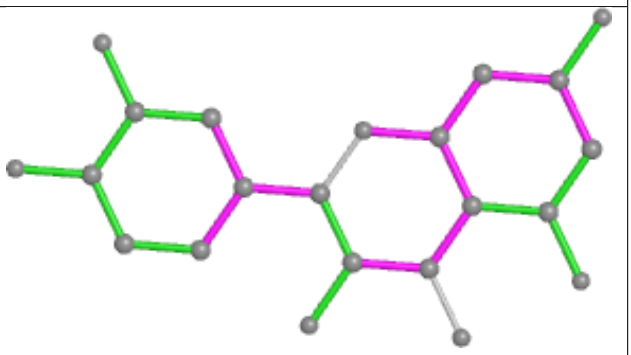


Rings

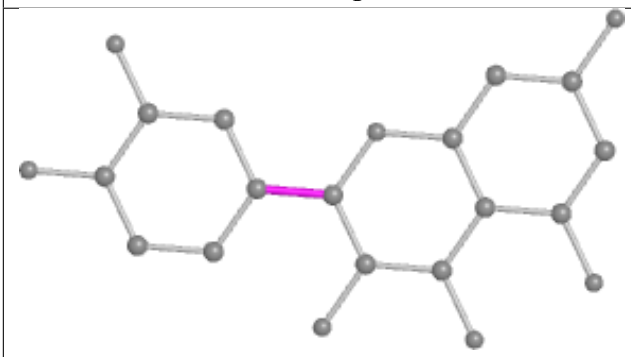
Ligand QUE C 1358



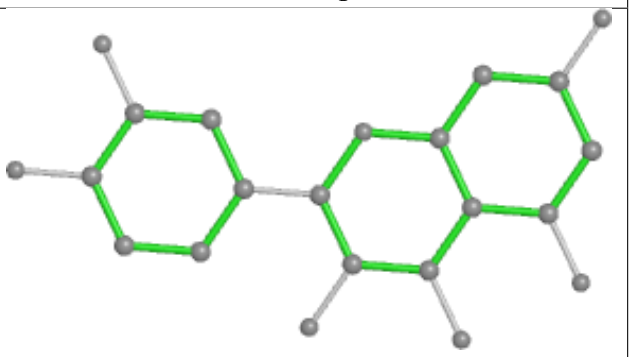
Bond lengths



Bond angles

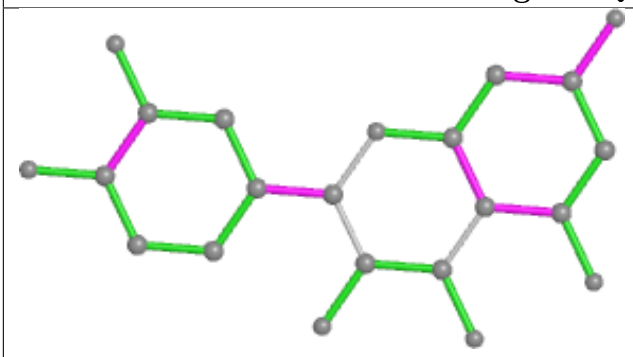


Torsions

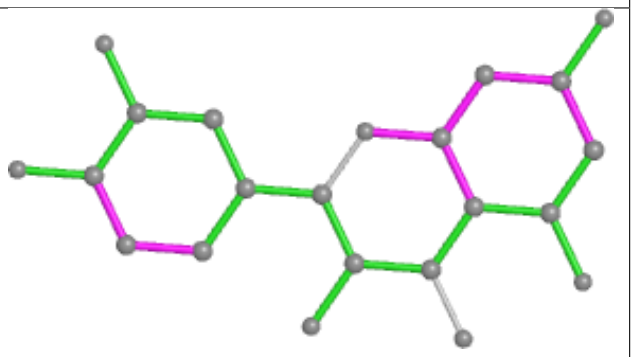


Rings

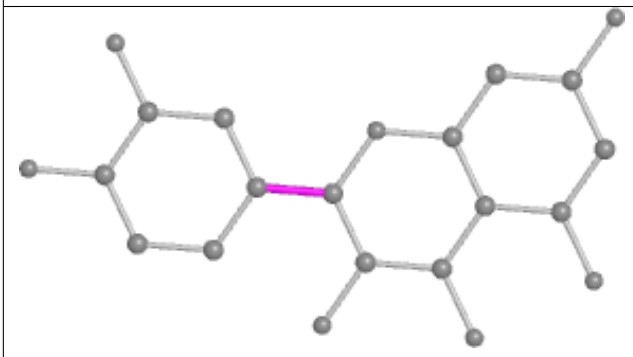
Ligand QUE A 1358



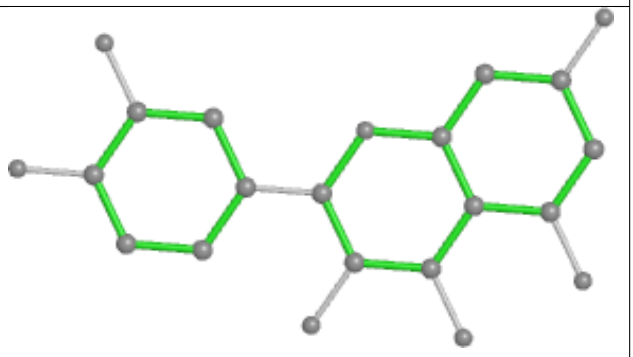
Bond lengths



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	344/350 (98%)	0.48	29 (8%) 11 14	7, 10, 18, 31	0
1	B	346/350 (98%)	0.52	35 (10%) 7 9	5, 10, 18, 41	0
1	C	343/350 (98%)	0.84	52 (15%) 2 3	6, 10, 18, 32	0
1	D	343/350 (98%)	0.71	46 (13%) 3 4	6, 10, 17, 34	0
All	All	1376/1400 (98%)	0.64	162 (11%) 4 6	5, 10, 18, 41	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	ILE	10.3
1	C	159	SER	8.4
1	C	160	SER	8.2
1	B	159	SER	7.9
1	D	159	SER	7.8
1	C	169	ILE	7.8
1	B	155	SER	7.0
1	D	160	SER	6.3
1	B	160	SER	6.2
1	B	3	SER	6.1
1	A	160	SER	6.0
1	B	168	THR	5.8
1	C	181	LEU	5.8
1	B	156	SER	5.8
1	D	169	ILE	5.5
1	C	168	THR	5.5
1	C	163	GLY	5.4
1	C	170	SER	5.3
1	C	289	ASP	5.2
1	C	165	ASP	5.2
1	C	197	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	4.9
1	B	167	SER	4.9
1	B	181	LEU	4.9
1	C	166	SER	4.8
1	D	262	THR	4.8
1	B	161	THR	4.7
1	A	169	ILE	4.7
1	B	170	SER	4.7
1	C	3	SER	4.7
1	A	90	ASN	4.6
1	C	164	PRO	4.6
1	B	162	THR	4.6
1	B	166	SER	4.6
1	D	4	SER	4.6
1	D	263	VAL	4.5
1	C	90	ASN	4.4
1	C	89	GLY	4.4
1	C	4	SER	4.4
1	A	161	THR	4.4
1	C	167	SER	4.4
1	D	181	LEU	4.3
1	B	187	THR	4.3
1	D	164	PRO	4.2
1	C	162	THR	4.2
1	B	164	PRO	4.2
1	D	166	SER	4.2
1	C	161	THR	4.1
1	B	163	GLY	4.1
1	D	289	ASP	4.0
1	D	168	THR	3.9
1	A	321	LEU	3.9
1	D	170	SER	3.9
1	B	278	VAL	3.8
1	C	321	LEU	3.8
1	C	171	THR	3.7
1	D	77	CYS	3.7
1	B	321	LEU	3.7
1	C	187	THR	3.7
1	D	264	THR	3.6
1	C	210	THR	3.6
1	C	178	TYR	3.6
1	C	182	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	321	LEU	3.6
1	D	350	TRP	3.5
1	A	78[A]	ASN	3.5
1	A	168	THR	3.4
1	A	278	VAL	3.4
1	D	171	THR	3.4
1	D	182	SER	3.4
1	D	320	VAL	3.4
1	C	184	THR	3.3
1	B	64	LEU	3.2
1	B	154	SER	3.2
1	B	197	ASN	3.2
1	A	320	VAL	3.2
1	D	161	THR	3.2
1	D	265	VAL	3.1
1	D	261	SER	3.1
1	D	154	SER	3.1
1	D	162	THR	3.1
1	A	159	SER	3.1
1	A	167	SER	3.1
1	D	167	SER	3.1
1	A	154	SER	3.0
1	A	77	CYS	3.0
1	B	76	TYR	3.0
1	C	262	THR	3.0
1	D	163	GLY	3.0
1	B	182	SER	3.0
1	C	327	SER	2.9
1	A	76	TYR	2.9
1	C	278	VAL	2.9
1	D	230	TYR	2.9
1	B	171	THR	2.9
1	A	181	LEU	2.8
1	D	278	VAL	2.8
1	B	320	VAL	2.8
1	C	67	ILE	2.8
1	A	323	VAL	2.8
1	D	76	TYR	2.7
1	C	241	ALA	2.7
1	D	50	LEU	2.7
1	D	165	ASP	2.7
1	C	88	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	261	SER	2.7
1	A	196	ALA	2.6
1	D	90	ASN	2.6
1	D	78	ASN	2.6
1	D	290	TYR	2.5
1	B	101	GLY	2.5
1	A	254	ILE	2.5
1	B	123[A]	MET	2.4
1	C	230	TYR	2.4
1	A	166	SER	2.4
1	C	179	ALA	2.4
1	C	264	THR	2.4
1	C	185	PRO	2.4
1	B	254	ILE	2.3
1	D	183	PHE	2.3
1	A	124	THR	2.3
1	C	189	THR	2.3
1	D	53	THR	2.3
1	D	187	THR	2.3
1	C	172	LEU	2.3
1	C	183	PHE	2.3
1	B	196	ALA	2.3
1	A	164	PRO	2.3
1	C	350	TRP	2.3
1	B	298	GLY	2.3
1	B	77	CYS	2.3
1	C	174	SER	2.3
1	C	77	CYS	2.3
1	D	338	GLY	2.3
1	C	333	ASN	2.3
1	A	50	LEU	2.2
1	D	101	GLY	2.2
1	C	92	THR	2.2
1	C	173	GLN	2.2
1	B	100[A]	SER	2.1
1	D	89	GLY	2.1
1	D	328	ASP	2.1
1	A	187	THR	2.1
1	C	50	LEU	2.1
1	D	124	THR	2.1
1	D	287	ILE	2.1
1	A	261	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	229	GLN	2.1
1	A	298	GLY	2.1
1	A	182	SER	2.1
1	B	124	THR	2.1
1	A	38	TYR	2.1
1	C	91	GLU	2.1
1	C	124	THR	2.0
1	A	275	ALA	2.0
1	C	328	ASP	2.0
1	C	109	ASN	2.0
1	A	100[A]	SER	2.0
1	D	123	MET	2.0
1	C	126	VAL	2.0
1	B	317	PHE	2.0
1	D	231	GLY	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)

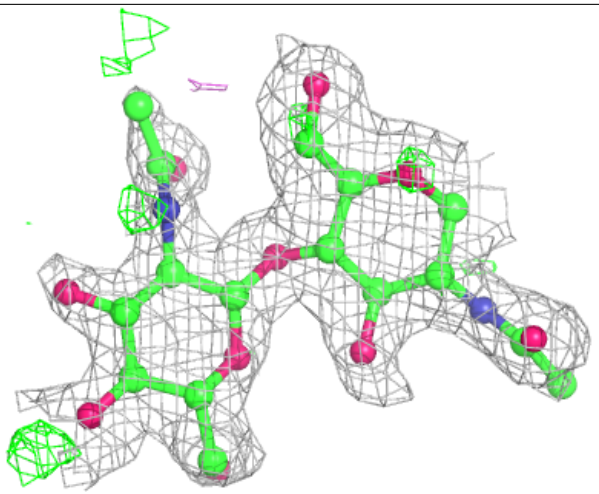
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

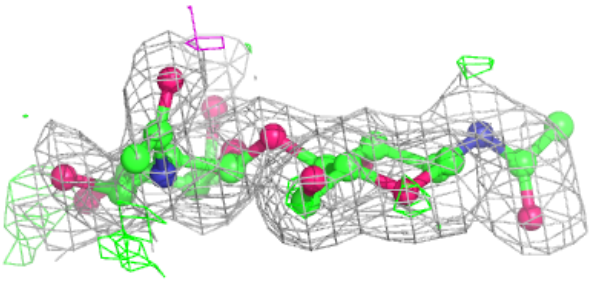
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.66	0.26	43,48,52,54	0
2	NAG	F	2	14/15	0.75	0.22	34,44,47,50	0
2	NAG	G	2	14/15	0.80	0.20	36,42,45,46	0
2	NAG	G	1	14/15	0.82	0.11	31,36,40,40	0
2	NAG	E	1	14/15	0.86	0.12	31,38,42,42	0
2	NAG	F	1	14/15	0.86	0.14	28,35,44,44	0

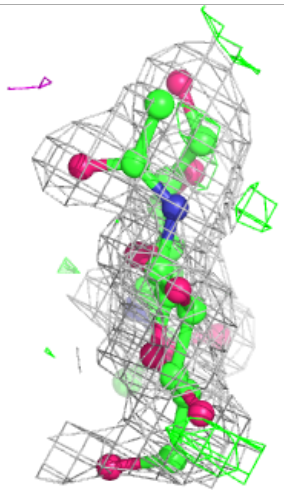
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

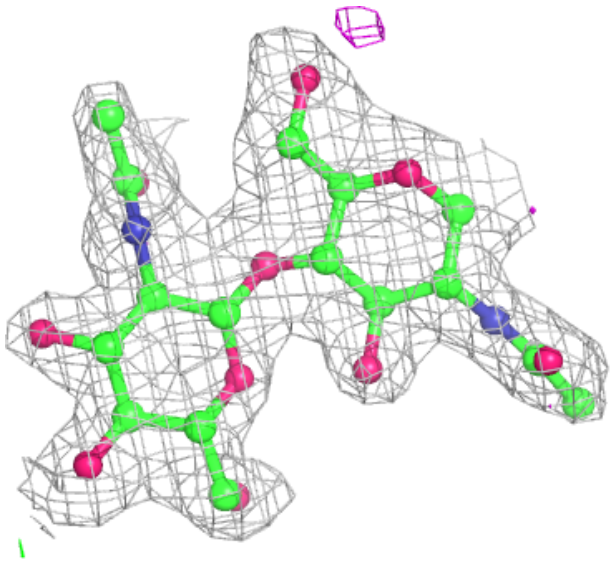


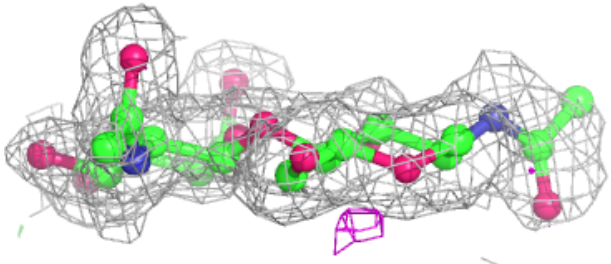


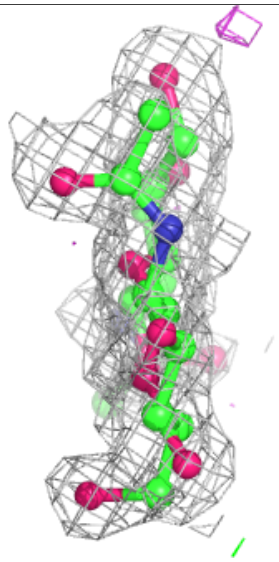


Electron density around Chain F:

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

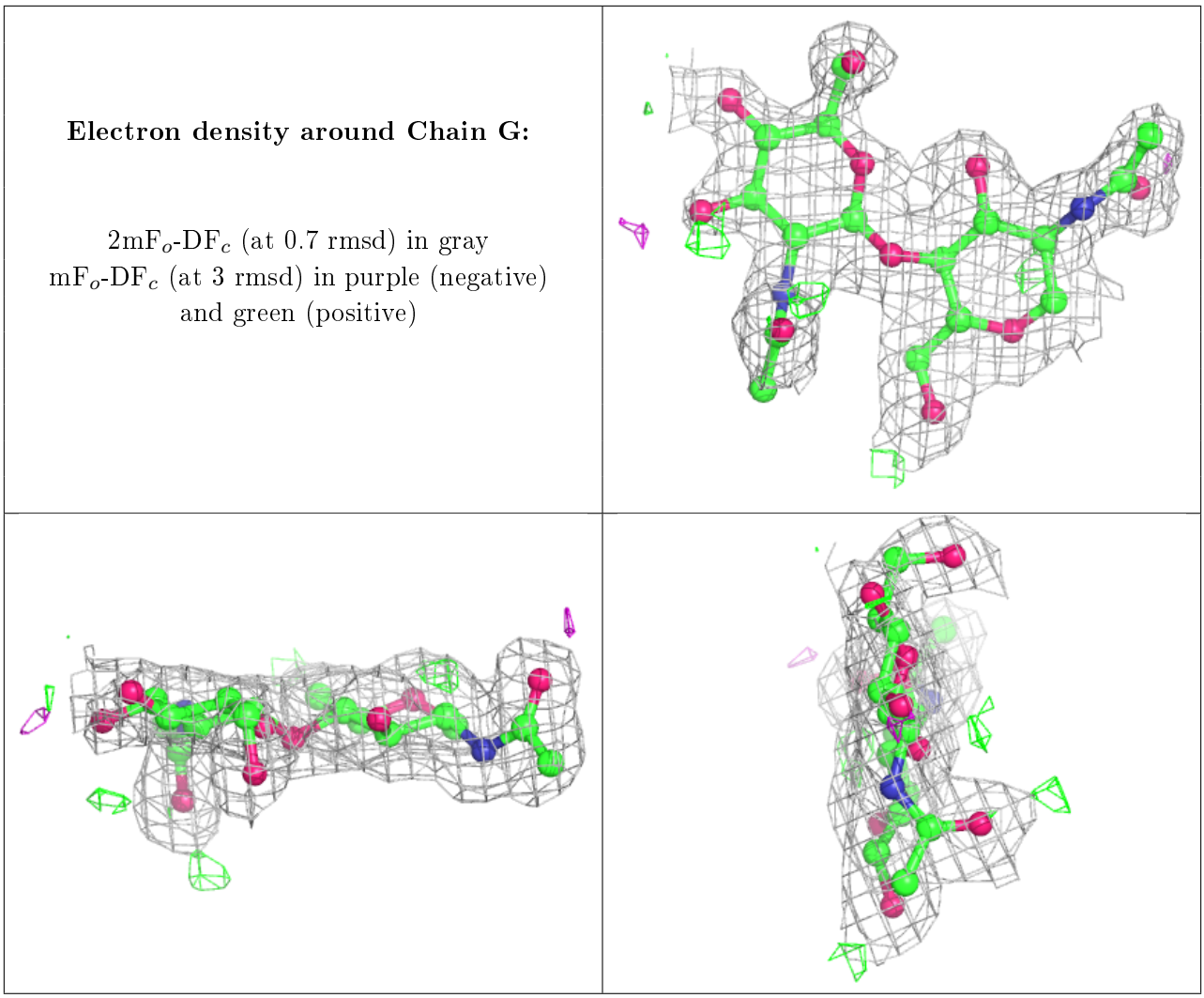






Electron density around Chain G:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
6	MPD	B	1358	8/8	0.70	0.31	34,41,44,45	0
3	NAG	A	1356	14/15	0.73	0.22	27,35,40,43	0
3	NAG	D	1351	14/15	0.82	0.21	39,44,50,50	0
3	NAG	A	1355	14/15	0.82	0.26	22,33,39,43	0
3	NAG	B	1352	14/15	0.83	0.19	36,44,49,49	0
6	MPD	C	1351	8/8	0.84	0.20	25,34,39,41	0
3	NAG	B	1353	14/15	0.84	0.18	26,35,45,48	0
6	MPD	A	1359	8/8	0.84	0.24	22,36,41,42	0
5	QUE	D	1357	22/22	0.85	0.14	16,20,23,26	0

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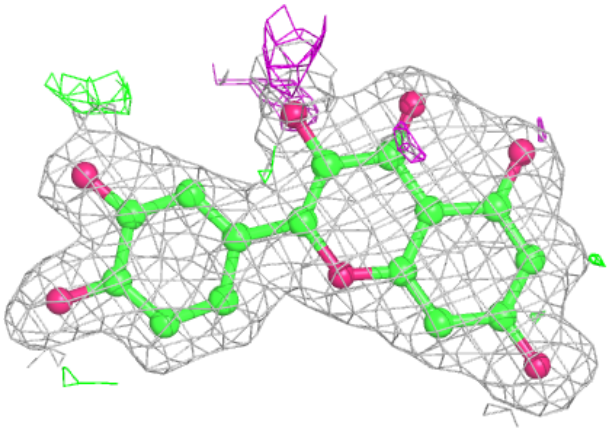
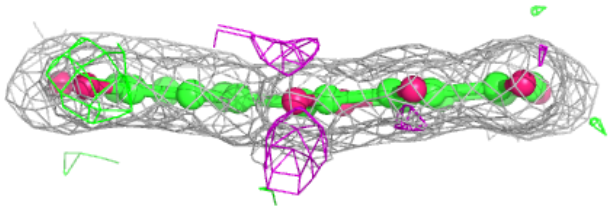
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	1355	14/15	0.85	0.13	30,36,46,47	0
6	MPD	B	1357	8/8	0.86	0.24	26,36,40,41	0
3	NAG	B	1354	14/15	0.86	0.13	32,39,45,46	0
3	NAG	C	1355	14/15	0.87	0.17	29,36,45,46	0
3	NAG	D	1354	14/15	0.87	0.15	26,30,38,39	0
5	QUE	A	1358	22/22	0.87	0.16	15,21,25,27	0
3	NAG	C	1356	14/15	0.88	0.12	31,40,46,47	0
3	NAG	A	1351	14/15	0.88	0.21	26,31,38,39	0
5	QUE	C	1358	22/22	0.89	0.11	14,18,22,25	0
5	QUE	B	1356	22/22	0.89	0.14	17,21,25,28	0
3	NAG	C	1352	14/15	0.90	0.16	29,36,43,45	0
3	NAG	B	1351	14/15	0.90	0.17	25,33,37,37	0
3	NAG	A	1354	14/15	0.91	0.11	22,28,39,39	0
4	CU	C	1357	1/1	0.97	0.10	17,17,17,17	1
4	CU	D	1356	1/1	0.98	0.11	18,18,18,18	1
4	CU	B	1355	1/1	0.99	0.07	17,17,17,17	1
4	CU	A	1357	1/1	0.99	0.06	19,19,19,19	1

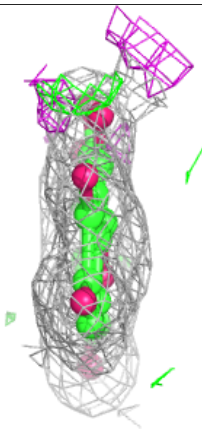
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QUE D 1357:

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

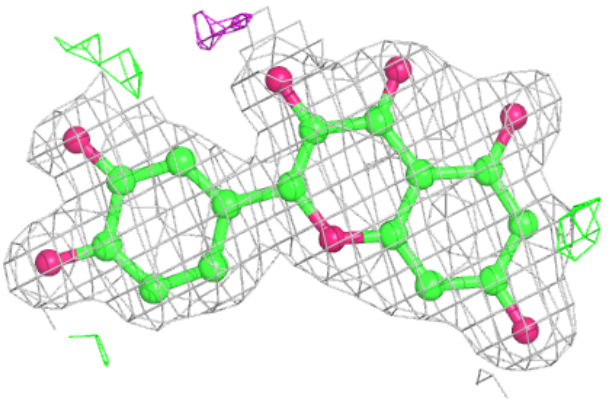


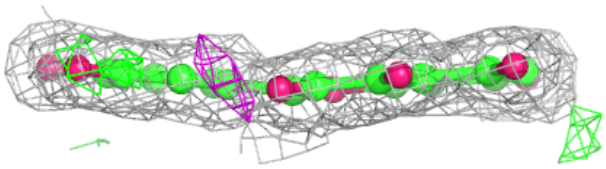


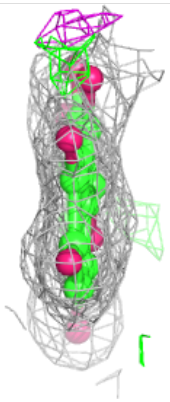


Electron density around QUE A 1358:

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

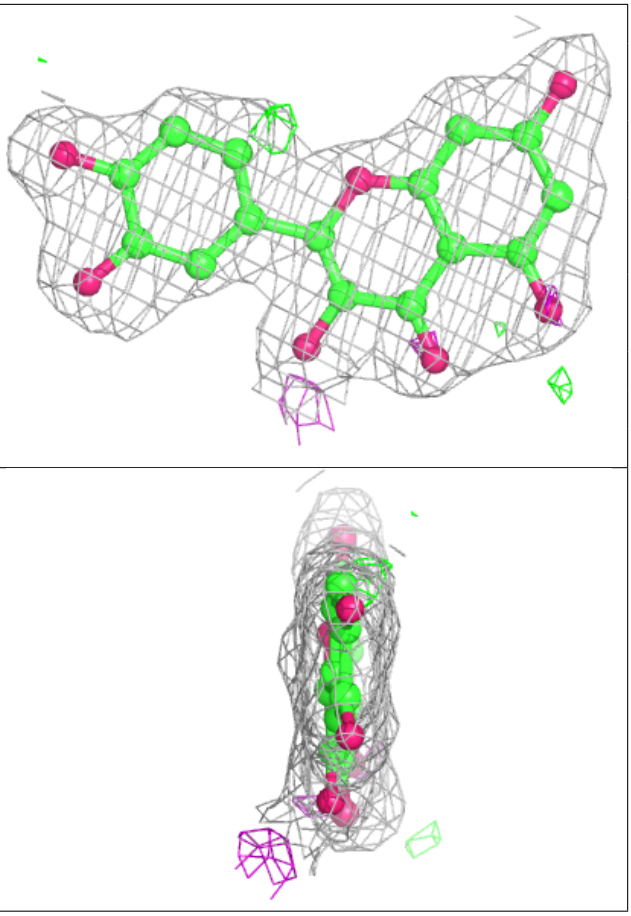






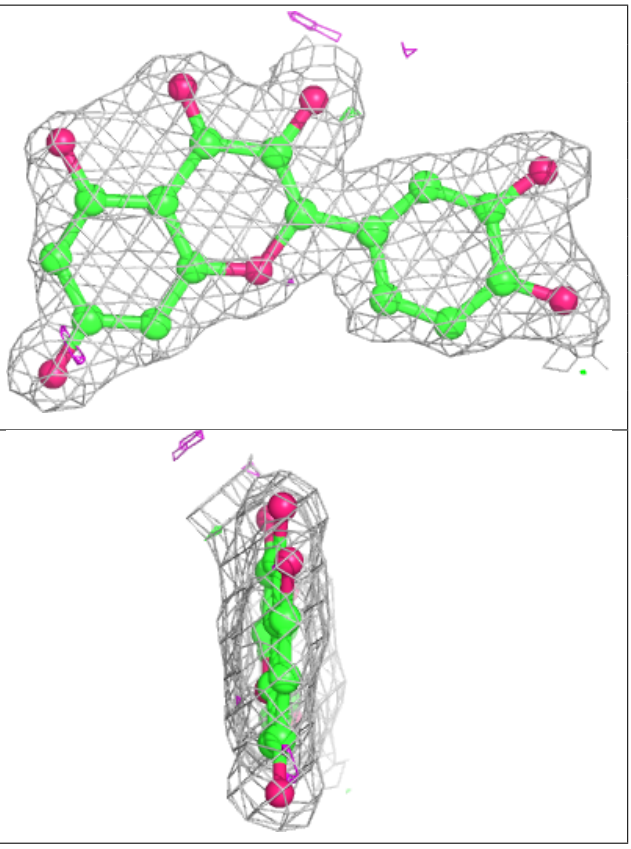
Electron density around QUE C 1358:

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



Electron density around QUE B 1356:

$2mF_o$-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.