Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2023 – 01:41 pm BST

PDB ID	:	8BHH
Title	:	The crystal structure of a feruloyl esterase C from Fusarium oxysporum in complex with p-coumaric acid
Authors	:	Dimarogona, M.; Topakas, E.; Kosinas, C.; Ferousi, C.; Nikolaivits, E.
Deposited on	:	2022-10-31
Resolution	:	1.69 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:

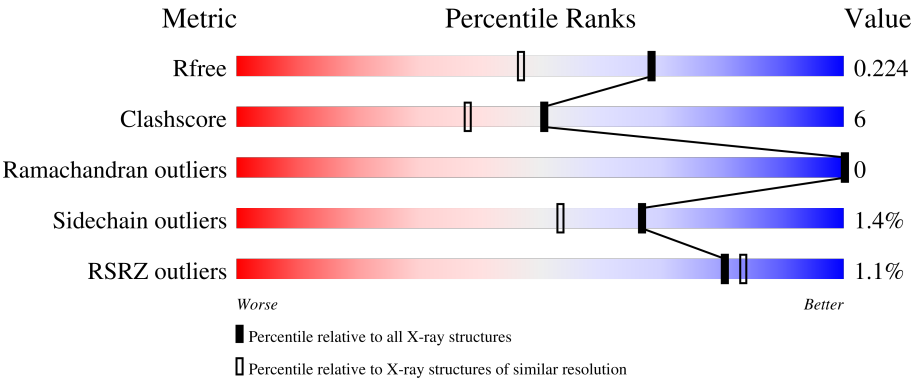
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	508	2%, 90%, 8%
1	B	508	88%, 10%
2	C	10	90%, 10%
2	G	10	100%
2	I	10	90%, 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	6	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	EDO	A	605	-	-	X	-
8	PG4	B	601	-	-	X	-
9	P6G	B	602	-	-	X	-

2 Entry composition

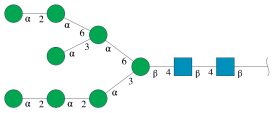
There are 11 unique types of molecules in this entry. The entry contains 9410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carboxylic ester hydrolase.

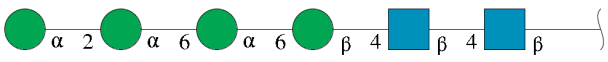
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	6	0
			3968	2506	690	751	21			
1	B	504	Total	C	N	O	S	0	7	0
			3970	2511	685	752	22			

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



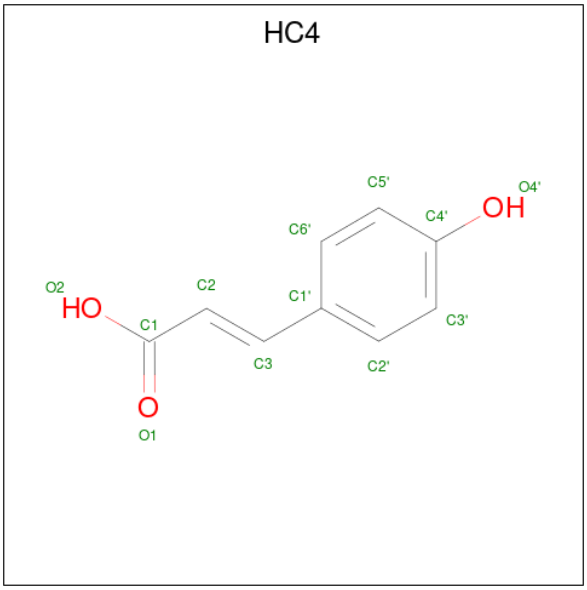
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			116	64	2	50			
2	G	10	Total	C	N	O	0	0	0
			116	64	2	50			
2	I	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



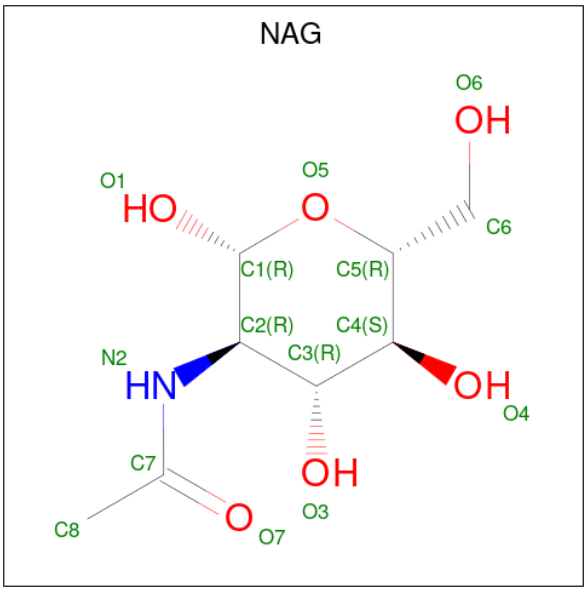
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: $C_9H_8O_3$) (labeled as "Ligand of Interest" by depositor).



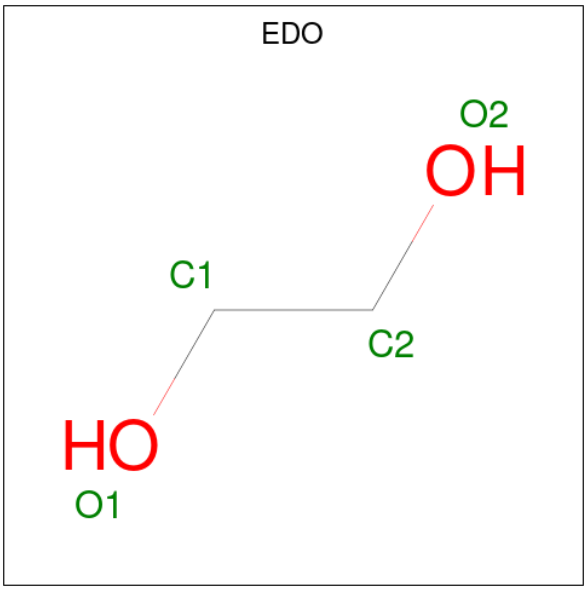
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

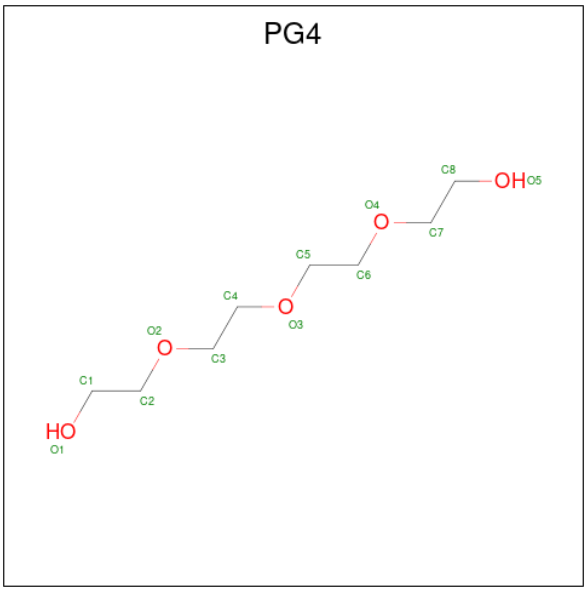


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

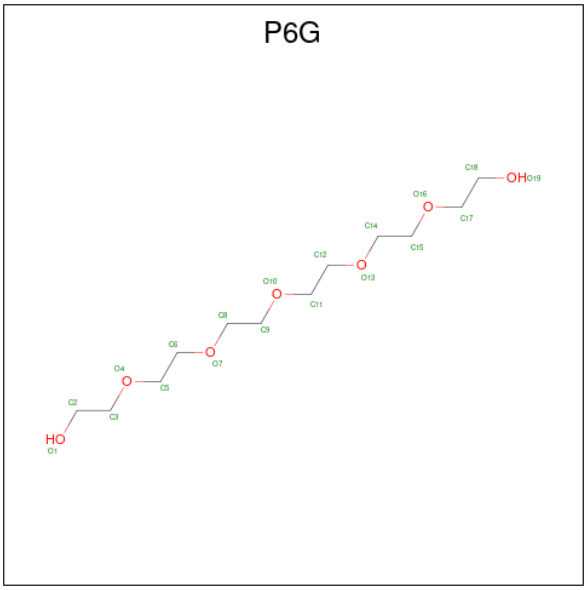
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



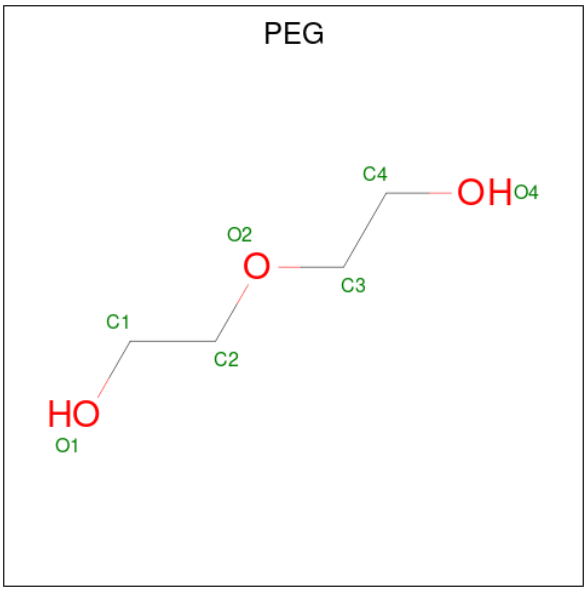
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 13 8 5	0	0

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 19 12 7	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 7 4 3	0	0

- Molecule 11 is water.

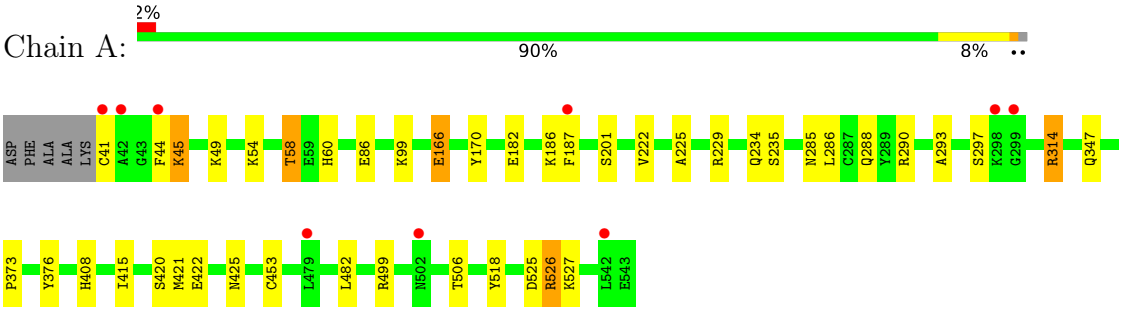
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	378	Total O 378 378	0	0
11	B	513	Total O 513 513	0	0

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.

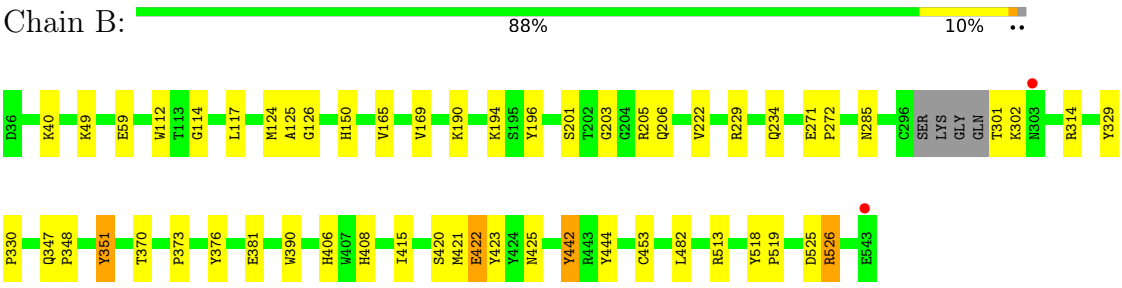
• Molecule 1: Carboxylic ester hydrolase

Chain A:



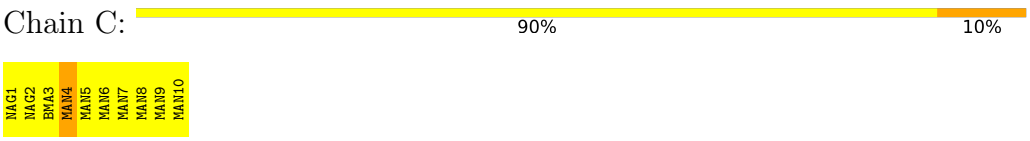
• Molecule 1: Carboxylic ester hydrolase

Chain B:



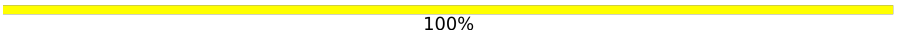
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



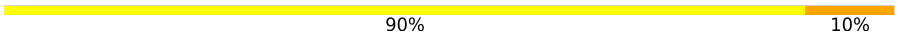
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



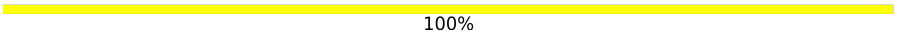
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.70Å 89.64Å 116.98Å 90.00° 103.99° 90.00°	Depositor
Resolution (Å)	113.51 – 1.69 113.51 – 1.69	Depositor EDS
% Data completeness (in resolution range)	69.5 (113.51-1.69) 69.5 (113.51-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.171 , 0.217 0.180 , 0.224	Depositor DCC
R_{free} test set	5158 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9410	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: CA, PEG, PG4, MAN, BMA, P6G, NAG, EDO, HC4

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	0.80	1/4080 (0.0%)	0.92	3/5543 (0.1%)
1	B	0.84	2/4088 (0.0%)	0.91	6/5554 (0.1%)
All	All	0.82	3/8168 (0.0%)	0.92	9/11097 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	GLU	CD-OE1	-7.01	1.18	1.25
1	B	381	GLU	CD-OE2	-5.21	1.20	1.25
1	A	166	GLU	CD-OE2	5.17	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	229	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	526	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	229	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	314	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	229	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	526	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	351	TYR	CB-CG-CD1	5.28	124.17	121.00
1	B	351	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	B	205	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	3968	0	3774	41	0
1	B	3970	0	3772	47	0
2	C	116	0	97	1	0
2	G	116	0	97	0	0
2	I	116	0	97	0	1
3	E	72	0	61	0	0
4	A	12	0	6	1	0
4	B	12	0	6	3	0
5	A	14	0	13	0	0
5	B	42	0	39	0	0
6	A	16	0	24	9	0
6	B	24	0	36	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	13	0	18	13	0
9	B	19	0	26	9	0
10	B	7	0	10	0	0
11	A	378	0	0	9	0
11	B	513	0	0	9	1
All	All	9410	0	8076	95	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 (95) 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)
11:A:736:HOH:O	9:B:602:P6G:H141	1.48	1.12
1:A:41:CYS:O	1:A:58:THR:HG21	1.74	0.87
8:B:601:PG4:H62	11:B:931:HOH:O	1.74	0.87
1:B:422:GLU:HG2	8:B:601:PG4:H71	1.60	0.84
6:A:605:EDO:O1	8:B:601:PG4:H82	1.85	0.76
1:B:314:ARG:HD3	9:B:602:P6G:H122	1.69	0.74
1:B:408:HIS:HD2	1:B:420:SER:OG	1.72	0.72
1:B:201[A]:SER:OG	4:B:604:HC4:C1	2.37	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASN:HD22	9:B:602:P6G:C17	2.05	0.70
1:A:425:ASN:HD22	9:B:602:P6G:H172	1.57	0.70
1:B:40:LYS:NZ	11:B:704:HOH:O	2.25	0.69
1:A:499:ARG:HD3	11:A:704:HOH:O	1.92	0.69
1:B:124[B]:MET:HE3	1:B:234:GLN:HE22	1.57	0.67
1:A:421[B]:MET:HE3	11:A:880:HOH:O	1.93	0.67
1:B:425:ASN:HD22	8:B:601:PG4:H72	1.60	0.67
8:B:601:PG4:H12	11:B:1107:HOH:O	1.96	0.65
1:A:499:ARG:CD	11:A:704:HOH:O	2.44	0.64
1:A:408:HIS:HD2	1:A:420:SER:OG	1.82	0.62
1:A:421[B]:MET:HG3	1:A:518:TYR:CZ	2.34	0.62
1:A:49:LYS:O	1:A:186:LYS:NZ	2.33	0.62
1:B:124[B]:MET:CE	1:B:234:GLN:HE22	2.12	0.62
1:A:285:ASN:HD21	1:A:421[B]:MET:HE1	1.65	0.61
1:B:201[B]:SER:OG	1:B:453:CYS:SG	2.59	0.61
1:A:293:ALA:HB1	6:A:606:EDO:H22	1.84	0.60
1:A:314:ARG:HH22	6:A:605:EDO:H12	1.66	0.59
1:B:59:GLU:CD	11:B:846:HOH:O	2.40	0.59
1:B:526:ARG:NH2	11:B:709:HOH:O	2.35	0.59
6:A:605:EDO:O1	8:B:601:PG4:C8	2.52	0.57
1:B:422:GLU:HA	8:B:601:PG4:H71	1.87	0.56
1:B:124[B]:MET:HE3	1:B:351:TYR:HB3	1.88	0.55
1:B:422:GLU:HA	8:B:601:PG4:C7	2.36	0.55
1:A:222:VAL:HG23	1:A:482:LEU:HD22	1.88	0.55
1:A:525:ASP:O	1:A:526:ARG:HB2	2.07	0.55
1:A:45:LYS:HG3	11:A:1003:HOH:O	2.06	0.55
1:A:314:ARG:HH22	6:A:605:EDO:C1	2.20	0.55
1:B:518:TYR:CD1	1:B:519:PRO:HA	2.42	0.54
1:A:285:ASN:HD21	1:A:421[B]:MET:CE	2.20	0.54
1:B:126:GLY:HA2	1:B:150:HIS:O	2.08	0.54
1:B:347:GLN:HB2	1:B:348:PRO:CD	2.38	0.53
1:B:222:VAL:HG23	1:B:482:LEU:HD22	1.91	0.53
1:B:285:ASN:HD21	1:B:421[B]:MET:CE	2.22	0.53
1:A:421[A]:MET:HG3	9:B:602:P6G:H181	1.91	0.52
1:A:422:GLU:HA	9:B:602:P6G:H151	1.92	0.52
1:B:112:TRP:CE2	1:B:114:GLY:HA2	2.45	0.52
1:A:506:THR:HG22	11:A:1012:HOH:O	2.09	0.51
1:B:525:ASP:O	1:B:526:ARG:HB2	2.10	0.51
1:A:288:GLN:C	6:A:605:EDO:H22	2.31	0.51
11:A:1078:HOH:O	2:C:4:MAN:H61	2.10	0.50
1:B:422:GLU:HG2	8:B:601:PG4:H61	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLN:HB2	1:B:348:PRO:HD2	1.94	0.50
1:A:297:SER:O	11:A:701:HOH:O	2.19	0.50
1:B:408:HIS:HE1	1:B:415:ILE:O	1.95	0.49
1:A:425:ASN:ND2	9:B:602:P6G:H172	2.24	0.49
1:B:124[B]:MET:CE	1:B:351:TYR:HB3	2.43	0.49
1:A:499:ARG:NE	11:A:704:HOH:O	2.47	0.47
1:A:201:SER:HA	1:A:225:ALA:O	2.15	0.46
1:A:44:PHE:CZ	1:A:187:PHE:HB2	2.51	0.46
1:A:60:HIS:NE2	1:A:86:GLU:OE1	2.47	0.46
1:A:201:SER:OG	1:A:453:CYS:SG	2.73	0.46
1:B:425:ASN:HD22	8:B:601:PG4:C7	2.28	0.46
1:A:290[B]:ARG:HG3	6:A:605:EDO:H11	1.97	0.45
1:A:373:PRO:HA	1:A:376:TYR:CD2	2.51	0.45
1:B:201[B]:SER:HB3	4:B:604:HC4:C1	2.46	0.45
1:A:166:GLU:OE1	1:A:170:TYR:OH	2.26	0.45
1:B:59:GLU:CG	11:B:846:HOH:O	2.64	0.45
1:A:408:HIS:HE1	1:A:415:ILE:O	1.99	0.45
1:B:370:THR:OG1	11:B:701:HOH:O	2.03	0.45
1:A:425:ASN:HD22	9:B:602:P6G:H171	1.80	0.45
1:A:314:ARG:HD3	8:B:601:PG4:H52	1.99	0.45
1:B:390:TRP:CZ3	1:B:423:TYR:HB2	2.52	0.45
1:B:421[A]:MET:HG3	1:B:518:TYR:CZ	2.52	0.45
1:A:421[B]:MET:HG2	9:B:602:P6G:C18	2.47	0.45
1:B:373:PRO:HA	1:B:376:TYR:CD2	2.52	0.44
1:A:286:LEU:N	1:A:286:LEU:HD23	2.32	0.44
1:B:190:LYS:NZ	6:B:607:EDO:H12	2.32	0.44
1:A:314:ARG:NH2	6:A:605:EDO:H12	2.30	0.43
1:A:408:HIS:CE1	1:A:415:ILE:O	2.71	0.43
1:B:442:TYR:CD1	1:B:442:TYR:C	2.90	0.43
1:B:329:TYR:CD1	1:B:330:PRO:HD2	2.54	0.43
1:B:201[A]:SER:OG	4:B:604:HC4:C2	2.66	0.42
1:A:235:SER:HB3	1:A:376:TYR:CD1	2.54	0.42
1:B:203:GLY:HA2	1:B:206:GLN:OE1	2.20	0.42
1:B:117:LEU:HA	1:B:196:TYR:O	2.20	0.42
8:B:601:PG4:H52	11:B:1127:HOH:O	2.20	0.42
1:B:271:GLU:N	1:B:272:PRO:CD	2.83	0.42
1:B:125:ALA:HA	1:B:126:GLY:HA3	1.93	0.41
1:B:112:TRP:CZ2	1:B:114:GLY:HA2	2.55	0.41
1:A:290[B]:ARG:HG3	6:A:605:EDO:C1	2.50	0.41
1:B:165:VAL:O	1:B:169:VAL:HG23	2.21	0.41
1:B:194:LYS:HE3	11:B:1103:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421[A]:MET:HG2	8:B:601:PG4:H81	2.03	0.40
1:B:421[B]:MET:HB3	1:B:421[B]:MET:HE2	1.72	0.40
1:B:124[B]:MET:CE	1:B:234:GLN:NE2	2.83	0.40
1:A:234:GLN:OE1	4:A:601:HC4:O4'	2.39	0.40
1:B:406:HIS:O	1:B:444:TYR:HA	2.21	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)
2:I:10:MAN:O6	11:B:1078:HOH:O[2_544]	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	507/508 (100%)	491 (97%)	16 (3%)	0	100	100
1	B	507/508 (100%)	497 (98%)	10 (2%)	0	100	100
All	All	1014/1016 (100%)	988 (97%)	26 (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	422/419 (101%)	415 (98%)	7 (2%)	60 46
1	B	423/419 (101%)	418 (99%)	5 (1%)	71 59
All	All	845/838 (101%)	833 (99%)	12 (1%)	67 53

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

Mol	Chain	Res	Type
1	A	45	LYS
1	A	54	LYS
1	A	58	THR
1	A	99	LYS
1	A	182	GLU
1	A	347	GLN
1	A	527	LYS
1	B	49	LYS
1	B	301	THR
1	B	302	LYS
1	B	442	TYR
1	B	513	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	285	ASN
1	A	408	HIS
1	A	425	ASN
1	B	234	GLN
1	B	285	ASN
1	B	408	HIS
1	B	435	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

36 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	C	1	2,1	14,14,15	1.00	1 (7%)	17,19,21	2.08	5 (29%)
2	MAN	C	10	2	11,11,12	0.84	0	15,15,17	1.46	2 (13%)
2	NAG	C	2	2	14,14,15	0.87	1 (7%)	17,19,21	1.56	3 (17%)
2	BMA	C	3	2	11,11,12	0.75	0	15,15,17	1.65	3 (20%)
2	MAN	C	4	2	11,11,12	1.08	2 (18%)	15,15,17	1.43	2 (13%)
2	MAN	C	5	2	11,11,12	0.90	1 (9%)	15,15,17	1.98	5 (33%)
2	MAN	C	6	2	11,11,12	0.82	0	15,15,17	2.25	4 (26%)
2	MAN	C	7	2	11,11,12	0.95	1 (9%)	15,15,17	2.22	4 (26%)
2	MAN	C	8	2	11,11,12	0.91	0	15,15,17	2.21	6 (40%)
2	MAN	C	9	2	11,11,12	1.26	0	15,15,17	2.72	4 (26%)
3	NAG	E	1	3,1	14,14,15	0.56	0	17,19,21	1.42	3 (17%)
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	1.50	4 (23%)
3	BMA	E	3	3	11,11,12	0.41	0	15,15,17	1.58	2 (13%)
3	MAN	E	4	3	11,11,12	0.80	0	15,15,17	1.76	4 (26%)
3	MAN	E	5	3	11,11,12	0.72	0	15,15,17	1.32	1 (6%)
3	MAN	E	6	3	11,11,12	1.32	2 (18%)	15,15,17	1.40	3 (20%)
2	NAG	G	1	2,1	14,14,15	1.03	2 (14%)	17,19,21	1.85	4 (23%)
2	MAN	G	10	2	11,11,12	1.42	2 (18%)	15,15,17	1.96	2 (13%)
2	NAG	G	2	2	14,14,15	0.77	0	17,19,21	1.77	4 (23%)
2	BMA	G	3	2	11,11,12	0.97	1 (9%)	15,15,17	1.90	4 (26%)
2	MAN	G	4	2	11,11,12	1.08	0	15,15,17	2.30	6 (40%)
2	MAN	G	5	2	11,11,12	1.08	0	15,15,17	1.69	2 (13%)
2	MAN	G	6	2	11,11,12	1.23	1 (9%)	15,15,17	2.04	6 (40%)
2	MAN	G	7	2	11,11,12	0.94	1 (9%)	15,15,17	2.21	5 (33%)
2	MAN	G	8	2	11,11,12	0.79	0	15,15,17	1.91	4 (26%)
2	MAN	G	9	2	11,11,12	0.64	0	15,15,17	1.60	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	I	1	2,1	14,14,15	0.93	1 (7%)	17,19,21	1.23	2 (11%)
2	MAN	I	10	2	11,11,12	0.64	0	15,15,17	2.33	7 (46%)
2	NAG	I	2	2	14,14,15	1.01	1 (7%)	17,19,21	2.28	4 (23%)
2	BMA	I	3	2	11,11,12	0.65	0	15,15,17	1.45	1 (6%)
2	MAN	I	4	2	11,11,12	0.81	0	15,15,17	1.49	3 (20%)
2	MAN	I	5	2	11,11,12	1.12	1 (9%)	15,15,17	2.12	3 (20%)
2	MAN	I	6	2	11,11,12	0.88	0	15,15,17	1.69	3 (20%)
2	MAN	I	7	2	11,11,12	0.55	0	15,15,17	1.94	4 (26%)
2	MAN	I	8	2	11,11,12	1.08	1 (9%)	15,15,17	2.28	5 (33%)
2	MAN	I	9	2	11,11,12	1.06	1 (9%)	15,15,17	1.84	4 (26%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	MAN	C	10	2	-	0/2/19/22	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	1/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	MAN	G	10	2	-	0/2/19/22	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	G	7	2	-	0/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1
2	MAN	G	9	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	MAN	I	10	2	-	2/2/19/22	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1
2	MAN	I	7	2	-	0/2/19/22	0/1/1/1
2	MAN	I	8	2	-	0/2/19/22	0/1/1/1
2	MAN	I	9	2	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	5	MAN	O5-C1	3.12	1.48	1.43
2	C	2	NAG	O5-C1	2.50	1.47	1.43
2	I	1	NAG	C1-C2	2.41	1.55	1.52
2	I	9	MAN	O4-C4	2.39	1.48	1.43
3	E	6	MAN	C1-C2	2.37	1.57	1.52
2	G	10	MAN	C2-C3	2.36	1.56	1.52
2	G	3	BMA	C2-C3	-2.33	1.49	1.52
2	I	8	MAN	O5-C1	2.33	1.47	1.43
2	G	6	MAN	O2-C2	2.25	1.48	1.43
2	I	2	NAG	O5-C5	2.24	1.48	1.43
2	G	1	NAG	O5-C1	2.21	1.47	1.43
2	C	1	NAG	O5-C1	-2.20	1.40	1.43
2	C	4	MAN	O4-C4	2.20	1.48	1.43
2	C	5	MAN	O5-C5	2.16	1.47	1.43
2	C	4	MAN	O5-C5	2.16	1.47	1.43
2	G	10	MAN	O5-C5	2.10	1.47	1.43
3	E	6	MAN	O4-C4	2.09	1.47	1.43
2	G	7	MAN	O2-C2	2.08	1.47	1.43
2	C	7	MAN	C1-C2	2.05	1.56	1.52
2	G	1	NAG	O5-C5	2.04	1.47	1.43

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	9	MAN	C1-C2-C3	7.04	118.31	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C1-O5-C5	-6.58	103.28	112.19
2	G	10	MAN	C1-O5-C5	6.17	120.56	112.19
2	C	7	MAN	C1-O5-C5	6.17	120.55	112.19
2	G	7	MAN	C1-C2-C3	-6.09	102.18	109.67
2	G	4	MAN	C1-C2-C3	5.84	116.85	109.67
2	G	1	NAG	O5-C5-C6	5.52	115.86	107.20
2	I	5	MAN	C1-C2-C3	5.08	115.91	109.67
2	C	9	MAN	O5-C5-C6	4.88	114.85	107.20
2	C	8	MAN	C1-O5-C5	4.74	118.62	112.19
2	C	1	NAG	O5-C1-C2	-4.66	103.92	111.29
2	I	3	BMA	C1-O5-C5	-4.66	105.88	112.19
2	I	8	MAN	C1-C2-C3	4.62	115.34	109.67
2	G	8	MAN	C1-C2-C3	4.49	115.19	109.67
2	C	5	MAN	C1-C2-C3	4.43	115.11	109.67
2	C	6	MAN	O2-C2-C1	-4.34	100.27	109.15
2	C	6	MAN	C1-O5-C5	4.32	118.04	112.19
2	C	6	MAN	C1-C2-C3	4.19	114.82	109.67
2	I	5	MAN	O5-C1-C2	-4.16	104.35	110.77
2	G	5	MAN	O4-C4-C3	-4.13	100.80	110.35
2	I	10	MAN	C6-C5-C4	-4.08	103.44	113.00
2	G	3	BMA	C1-O5-C5	-4.04	106.72	112.19
3	E	3	BMA	C1-O5-C5	4.02	117.64	112.19
2	I	8	MAN	C1-O5-C5	4.02	117.63	112.19
2	G	3	BMA	O5-C5-C6	4.01	113.49	107.20
2	G	6	MAN	O3-C3-C2	-4.00	102.34	109.99
2	I	7	MAN	O5-C5-C6	3.99	113.45	107.20
2	G	4	MAN	C1-O5-C5	3.93	117.52	112.19
2	I	9	MAN	O5-C1-C2	3.92	116.82	110.77
2	C	9	MAN	O2-C2-C3	-3.88	102.37	110.14
2	G	6	MAN	C1-C2-C3	-3.86	104.92	109.67
3	E	5	MAN	O5-C5-C6	3.83	113.21	107.20
3	E	4	MAN	O5-C1-C2	-3.75	104.98	110.77
2	I	7	MAN	O2-C2-C1	-3.75	101.47	109.15
2	G	8	MAN	O3-C3-C2	-3.65	103.01	109.99
2	I	7	MAN	C1-O5-C5	3.63	117.11	112.19
2	C	3	BMA	C1-C2-C3	-3.63	105.21	109.67
2	I	6	MAN	O5-C5-C6	3.59	112.83	107.20
2	G	2	NAG	C1-O5-C5	-3.58	107.34	112.19
2	G	10	MAN	C1-C2-C3	3.58	114.06	109.67
2	I	8	MAN	O3-C3-C2	-3.57	103.15	109.99
2	I	5	MAN	C1-O5-C5	3.57	117.03	112.19
3	E	1	NAG	O5-C5-C6	3.57	112.80	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	O5-C5-C6	3.55	112.78	107.20
2	G	2	NAG	C4-C3-C2	-3.52	105.87	111.02
2	C	1	NAG	C1-O5-C5	3.49	116.92	112.19
2	C	5	MAN	O3-C3-C2	-3.44	103.41	109.99
2	I	9	MAN	O2-C2-C1	-3.43	102.13	109.15
2	C	8	MAN	O2-C2-C1	-3.35	102.30	109.15
2	C	7	MAN	O5-C1-C2	-3.34	105.62	110.77
2	C	8	MAN	O3-C3-C2	-3.34	103.61	109.99
2	I	10	MAN	O5-C5-C6	3.30	112.38	107.20
2	I	10	MAN	C1-O5-C5	3.28	116.63	112.19
2	C	10	MAN	C1-C2-C3	3.26	113.67	109.67
2	I	10	MAN	C2-C3-C4	-3.24	105.28	110.89
2	I	6	MAN	C1-O5-C5	3.22	116.56	112.19
2	G	9	MAN	O5-C5-C4	-3.19	103.08	110.83
2	G	9	MAN	O2-C2-C1	-3.11	102.79	109.15
2	C	6	MAN	O5-C5-C6	3.09	112.06	107.20
2	C	1	NAG	C1-C2-N2	-3.07	105.24	110.49
2	C	5	MAN	O5-C5-C6	2.97	111.86	107.20
2	G	2	NAG	O4-C4-C3	-2.97	103.49	110.35
3	E	2	NAG	C3-C4-C5	2.96	115.53	110.24
2	C	3	BMA	C2-C3-C4	2.92	115.95	110.89
2	C	2	NAG	C1-O5-C5	-2.90	108.26	112.19
2	C	2	NAG	C4-C3-C2	-2.88	106.80	111.02
2	C	4	MAN	O4-C4-C5	2.83	116.33	109.30
2	I	10	MAN	O3-C3-C4	-2.81	103.85	110.35
2	G	7	MAN	O5-C1-C2	-2.76	106.52	110.77
2	G	1	NAG	O4-C4-C3	-2.72	104.06	110.35
2	G	5	MAN	C1-O5-C5	2.72	115.88	112.19
2	I	9	MAN	C1-C2-C3	-2.70	106.34	109.67
2	C	9	MAN	O2-C2-C1	-2.68	103.67	109.15
2	C	4	MAN	C6-C5-C4	-2.62	106.88	113.00
2	I	7	MAN	C6-C5-C4	-2.62	106.88	113.00
3	E	4	MAN	O3-C3-C2	-2.60	105.01	109.99
2	C	2	NAG	C3-C4-C5	2.60	114.88	110.24
2	I	4	MAN	O4-C4-C5	2.58	115.71	109.30
2	I	10	MAN	C1-C2-C3	2.58	112.83	109.67
2	C	5	MAN	O4-C4-C3	-2.57	104.40	110.35
2	C	7	MAN	C6-C5-C4	-2.52	107.09	113.00
2	C	3	BMA	O4-C4-C3	-2.50	104.57	110.35
2	C	5	MAN	O2-C2-C3	-2.50	105.14	110.14
2	C	8	MAN	O2-C2-C3	2.50	115.14	110.14
2	G	8	MAN	C1-O5-C5	2.47	115.54	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3	BMA	C2-C3-C4	-2.47	106.62	110.89
2	I	10	MAN	O6-C6-C5	-2.46	102.85	111.29
2	G	4	MAN	C6-C5-C4	-2.45	107.27	113.00
2	C	8	MAN	C2-C3-C4	2.45	115.13	110.89
2	I	1	NAG	C1-O5-C5	-2.45	108.88	112.19
2	G	6	MAN	O5-C1-C2	2.43	114.52	110.77
2	I	2	NAG	C8-C7-N2	-2.43	111.99	116.10
2	G	6	MAN	O4-C4-C3	-2.40	104.80	110.35
3	E	4	MAN	C1-C2-C3	2.40	112.61	109.67
2	C	7	MAN	C1-C2-C3	2.39	112.60	109.67
2	C	1	NAG	O3-C3-C2	2.38	114.40	109.47
2	G	8	MAN	O2-C2-C3	-2.37	105.39	110.14
3	E	2	NAG	C1-O5-C5	2.36	115.40	112.19
2	G	1	NAG	C6-C5-C4	-2.36	107.48	113.00
3	E	3	BMA	O2-C2-C3	2.36	114.86	110.14
3	E	6	MAN	C1-C2-C3	2.34	112.55	109.67
2	C	1	NAG	C2-N2-C7	2.34	126.23	122.90
2	G	7	MAN	O3-C3-C2	-2.32	105.54	109.99
2	G	4	MAN	O5-C1-C2	-2.32	107.19	110.77
2	G	6	MAN	C1-O5-C5	-2.32	109.05	112.19
2	I	9	MAN	O3-C3-C4	-2.30	105.02	110.35
2	I	6	MAN	C1-C2-C3	2.27	112.46	109.67
2	C	8	MAN	O5-C1-C2	-2.27	107.27	110.77
2	G	6	MAN	O4-C4-C5	2.27	114.93	109.30
2	I	1	NAG	O3-C3-C4	2.26	115.58	110.35
3	E	2	NAG	O3-C3-C2	-2.25	104.81	109.47
2	G	2	NAG	O6-C6-C5	-2.23	103.65	111.29
2	G	9	MAN	C3-C4-C5	-2.21	106.29	110.24
2	I	4	MAN	O4-C4-C3	-2.21	105.23	110.35
3	E	6	MAN	O5-C5-C6	2.21	110.67	107.20
2	I	8	MAN	C6-C5-C4	-2.20	107.85	113.00
2	G	1	NAG	C1-O5-C5	-2.19	109.22	112.19
2	I	2	NAG	C6-C5-C4	-2.18	107.89	113.00
2	G	4	MAN	C2-C3-C4	-2.17	107.14	110.89
2	I	4	MAN	C1-O5-C5	2.16	115.11	112.19
3	E	1	NAG	O3-C3-C4	2.15	115.33	110.35
3	E	6	MAN	O5-C1-C2	-2.13	107.48	110.77
3	E	1	NAG	O4-C4-C5	-2.12	104.03	109.30
2	G	7	MAN	O5-C5-C4	-2.08	105.76	110.83
2	I	8	MAN	C3-C4-C5	-2.08	106.53	110.24
3	E	2	NAG	O7-C7-C8	-2.06	118.22	122.06
2	G	4	MAN	C3-C4-C5	-2.06	106.56	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	10	MAN	C1-O5-C5	2.04	114.96	112.19
3	E	4	MAN	C2-C3-C4	2.04	114.42	110.89
2	G	3	BMA	O5-C5-C4	-2.03	105.88	110.83
2	G	7	MAN	O2-C2-C3	2.02	114.18	110.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	10	MAN	O5-C5-C6-O6
2	I	10	MAN	C4-C5-C6-O6
2	C	9	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	9	MAN	O5-C5-C6-O6
2	I	5	MAN	O5-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
2	I	5	MAN	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

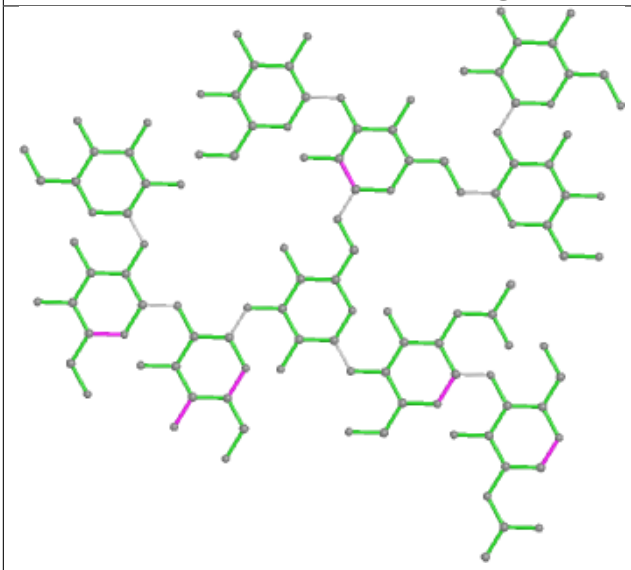
There are no ring outliers.

2 monomers are involved in 2 short contacts:

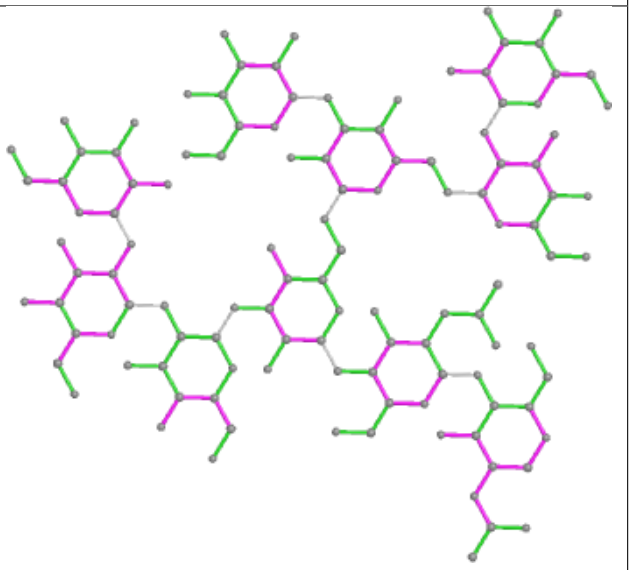
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	10	MAN	0	1
2	C	4	MAN	1	0

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

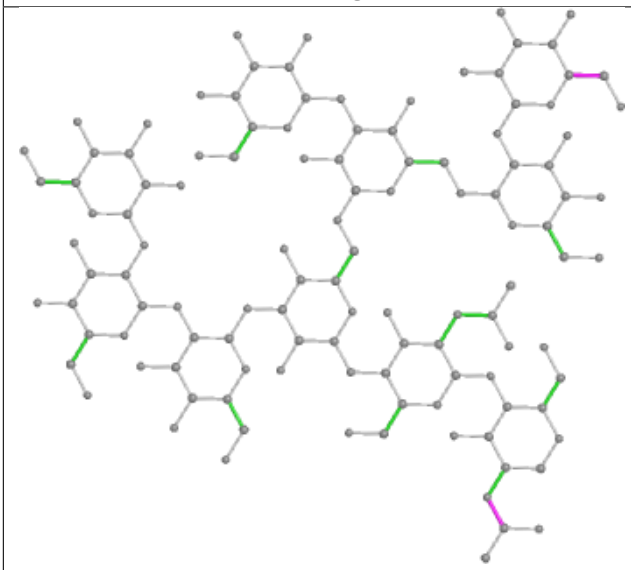
Oligosaccharide Chain C



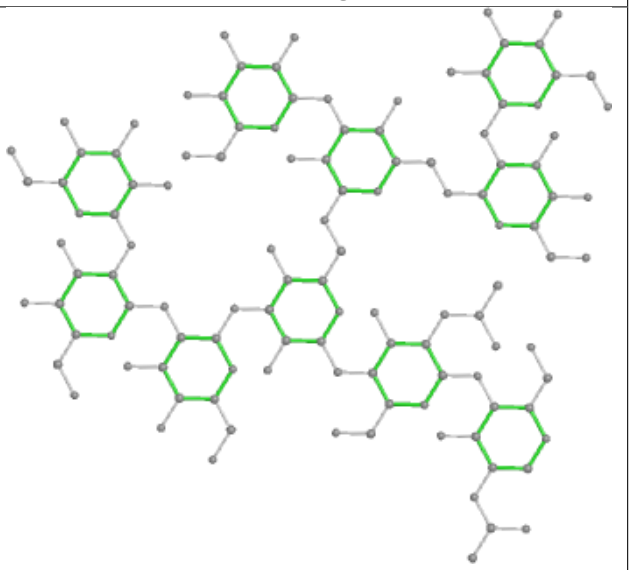
Bond lengths



Bond angles

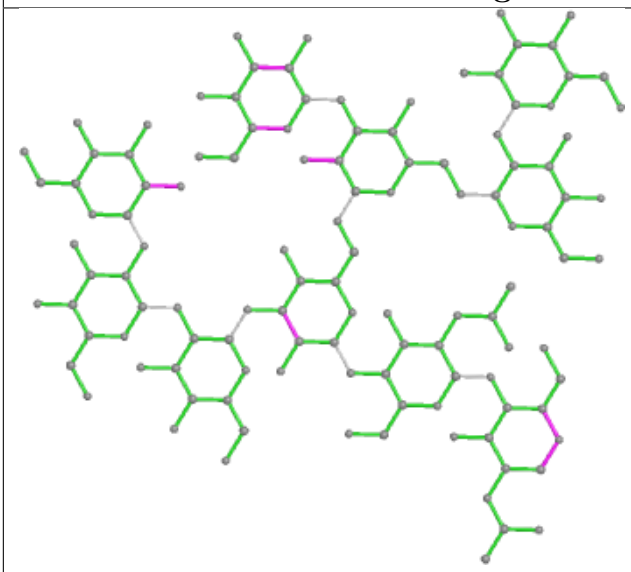


Torsions

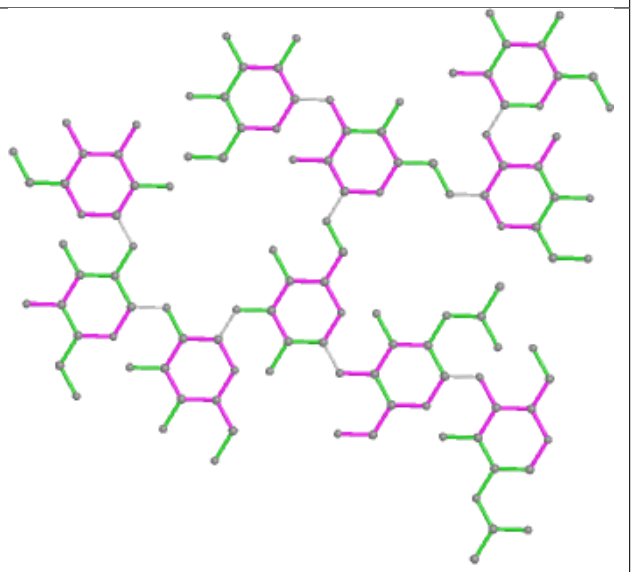


Rings

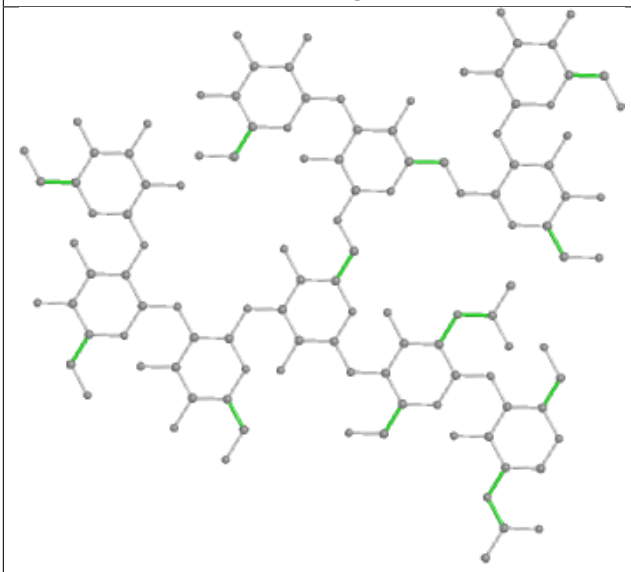
Oligosaccharide Chain G



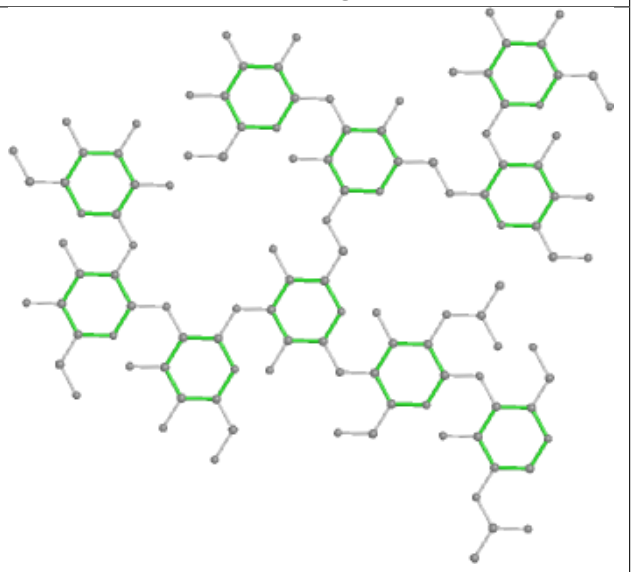
Bond lengths



Bond angles

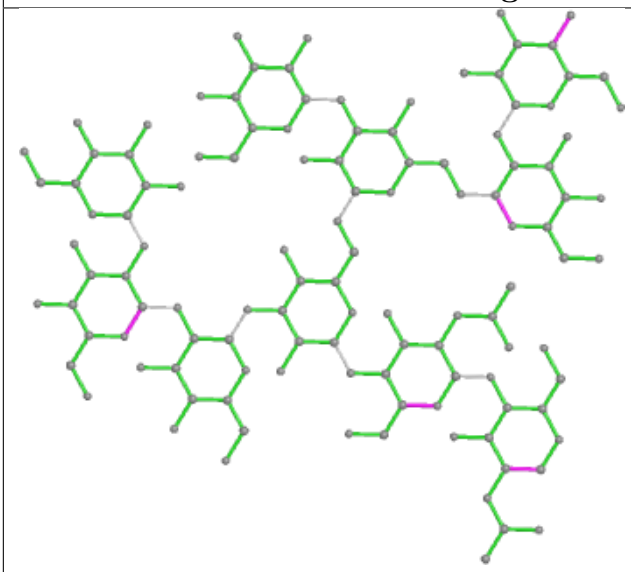


Torsions

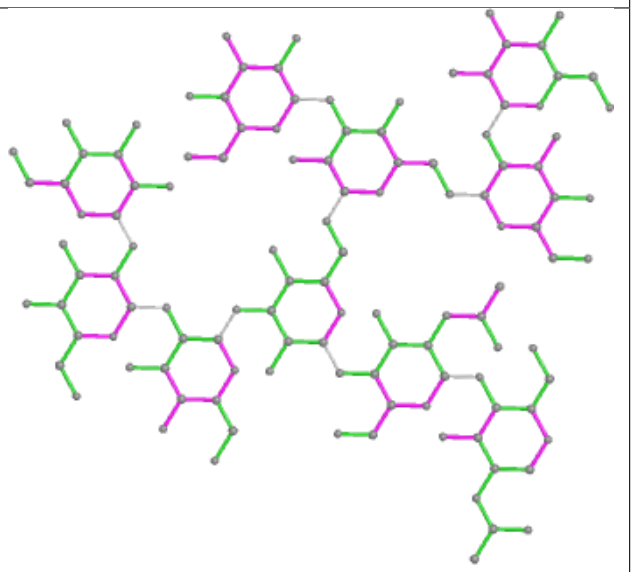


Rings

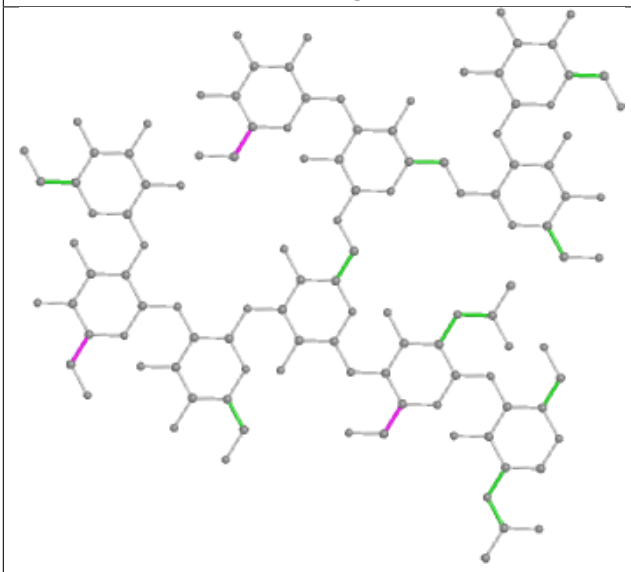
Oligosaccharide Chain I



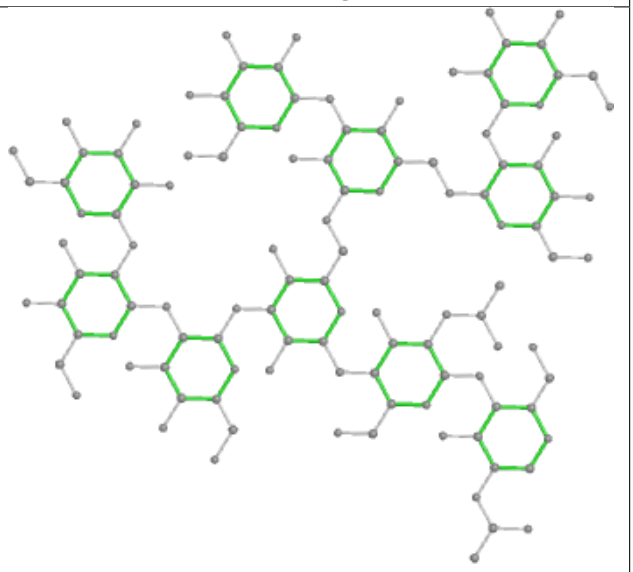
Bond lengths



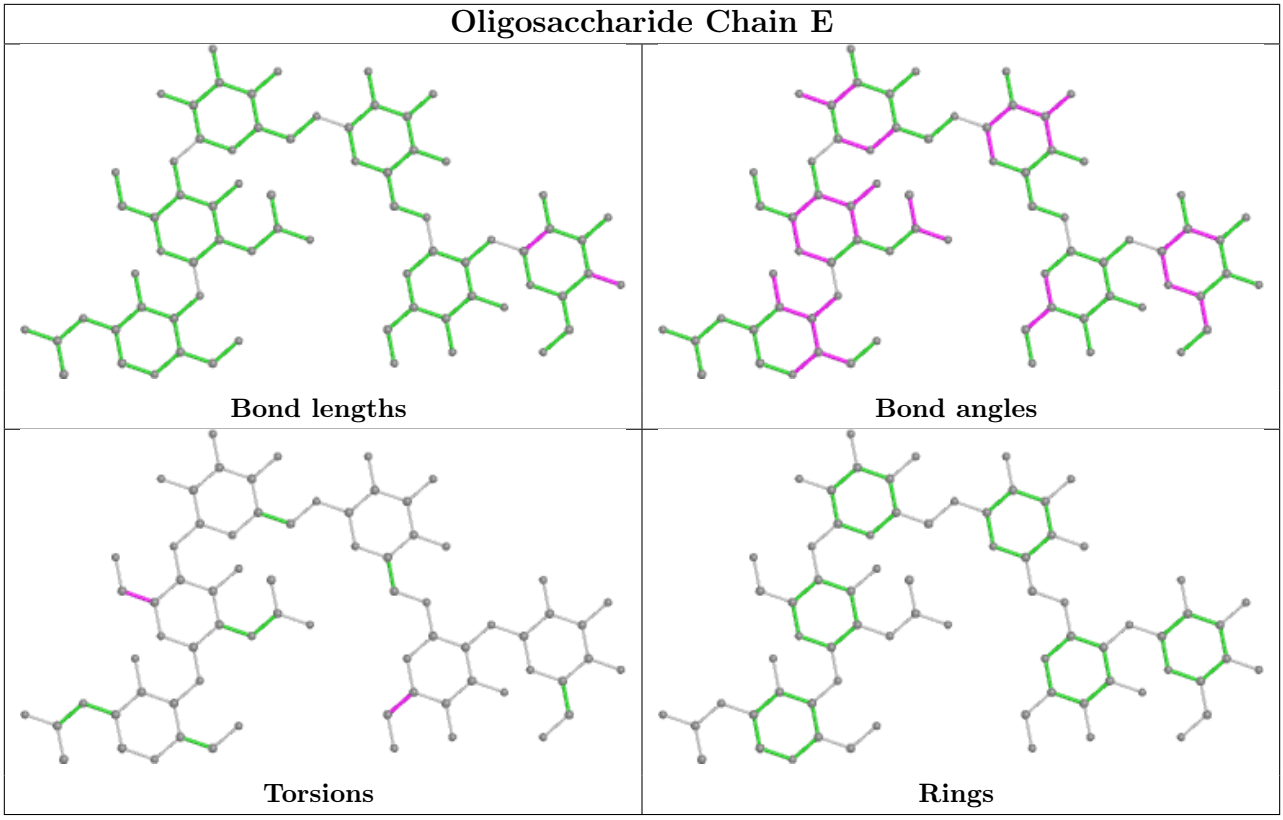
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
6	EDO	A	606	-	3,3,3	0.28	0	2,2,2	0.16	0
10	PEG	B	609	-	6,6,6	0.28	0	5,5,5	0.19	0
6	EDO	B	608	-	3,3,3	0.52	0	2,2,2	0.63	0
6	EDO	B	605	-	3,3,3	0.20	0	2,2,2	0.40	0
6	EDO	B	607	-	3,3,3	0.35	0	2,2,2	0.53	0
6	EDO	A	604	-	3,3,3	0.26	0	2,2,2	0.45	0
4	HC4	B	604	-	12,12,12	0.84	1 (8%)	15,15,15	0.58	0
6	EDO	B	613	-	3,3,3	0.11	0	2,2,2	0.26	0
6	EDO	B	606	-	3,3,3	0.37	0	2,2,2	0.72	0
5	NAG	B	612	1	14,14,15	0.75	0	17,19,21	1.68	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	603	-	3,3,3	0.32	0	2,2,2	0.44	0
6	EDO	A	605	-	3,3,3	0.61	0	2,2,2	0.59	0
8	PG4	B	601	-	12,12,12	0.57	0	11,11,11	0.60	0
4	HC4	A	601	-	12,12,12	0.93	0	15,15,15	0.43	0
5	NAG	B	611	1	14,14,15	0.74	0	17,19,21	1.39	2 (11%)
5	NAG	B	603	1	14,14,15	0.85	1 (7%)	17,19,21	1.35	4 (23%)
6	EDO	B	610	-	3,3,3	0.19	0	2,2,2	0.23	0
9	P6G	B	602	-	18,18,18	0.25	0	17,17,17	0.35	0
5	NAG	A	602	1	14,14,15	0.88	0	17,19,21	1.10	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	606	-	-	1/1/1/1	-
10	PEG	B	609	-	-	1/4/4/4	-
6	EDO	B	608	-	-	1/1/1/1	-
6	EDO	B	605	-	-	1/1/1/1	-
6	EDO	B	607	-	-	1/1/1/1	-
6	EDO	A	604	-	-	1/1/1/1	-
4	HC4	B	604	-	-	0/5/5/5	0/1/1/1
6	EDO	B	613	-	-	1/1/1/1	-
6	EDO	B	606	-	-	0/1/1/1	-
5	NAG	B	612	1	-	1/6/23/26	0/1/1/1
6	EDO	A	603	-	-	1/1/1/1	-
6	EDO	A	605	-	-	1/1/1/1	-
8	PG4	B	601	-	-	6/10/10/10	-
4	HC4	A	601	-	-	2/5/5/5	0/1/1/1
5	NAG	B	611	1	-	2/6/23/26	0/1/1/1
5	NAG	B	603	1	-	0/6/23/26	0/1/1/1
6	EDO	B	610	-	-	1/1/1/1	-
9	P6G	B	602	-	-	8/16/16/16	-
5	NAG	A	602	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	HC4	O1-C1	2.20	1.28	1.23
5	B	603	NAG	C3-C2	2.11	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	612	NAG	C1-O5-C5	5.29	119.36	112.19
5	B	612	NAG	C1-C2-N2	-3.15	105.11	110.49
5	B	603	NAG	O3-C3-C2	-2.94	103.39	109.47
5	B	611	NAG	O5-C5-C6	2.72	111.47	107.20
5	B	611	NAG	C1-C2-N2	2.49	114.74	110.49
5	B	603	NAG	C8-C7-N2	-2.34	112.14	116.10
5	A	602	NAG	C4-C3-C2	2.18	114.22	111.02
5	B	603	NAG	O7-C7-C8	2.02	125.81	122.06
5	B	603	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	601	PG4	C3-C4-O3-C5
9	B	602	P6G	O7-C8-C9-O10
9	B	602	P6G	O10-C11-C12-O13
10	B	609	PEG	O1-C1-C2-O2
9	B	602	P6G	O16-C17-C18-O19
6	A	603	EDO	O1-C1-C2-O2
6	A	606	EDO	O1-C1-C2-O2
6	B	608	EDO	O1-C1-C2-O2
6	B	610	EDO	O1-C1-C2-O2
8	B	601	PG4	O2-C3-C4-O3
9	B	602	P6G	O13-C14-C15-O16
6	B	607	EDO	O1-C1-C2-O2
5	B	612	NAG	C8-C7-N2-C2
5	B	611	NAG	O5-C5-C6-O6
9	B	602	P6G	C8-C9-O10-C11
5	B	611	NAG	C4-C5-C6-O6
9	B	602	P6G	C9-C8-O7-C6
8	B	601	PG4	C1-C2-O2-C3
6	B	613	EDO	O1-C1-C2-O2
8	B	601	PG4	C5-C6-O4-C7
9	B	602	P6G	C15-C14-O13-C12
8	B	601	PG4	C6-C5-O3-C4
6	A	605	EDO	O1-C1-C2-O2
9	B	602	P6G	C2-C3-O4-C5
8	B	601	PG4	C8-C7-O4-C6
4	A	601	HC4	C6'-C1'-C3-C2
4	A	601	HC4	C2'-C1'-C3-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	604	EDO	O1-C1-C2-O2
6	B	605	EDO	O1-C1-C2-O2

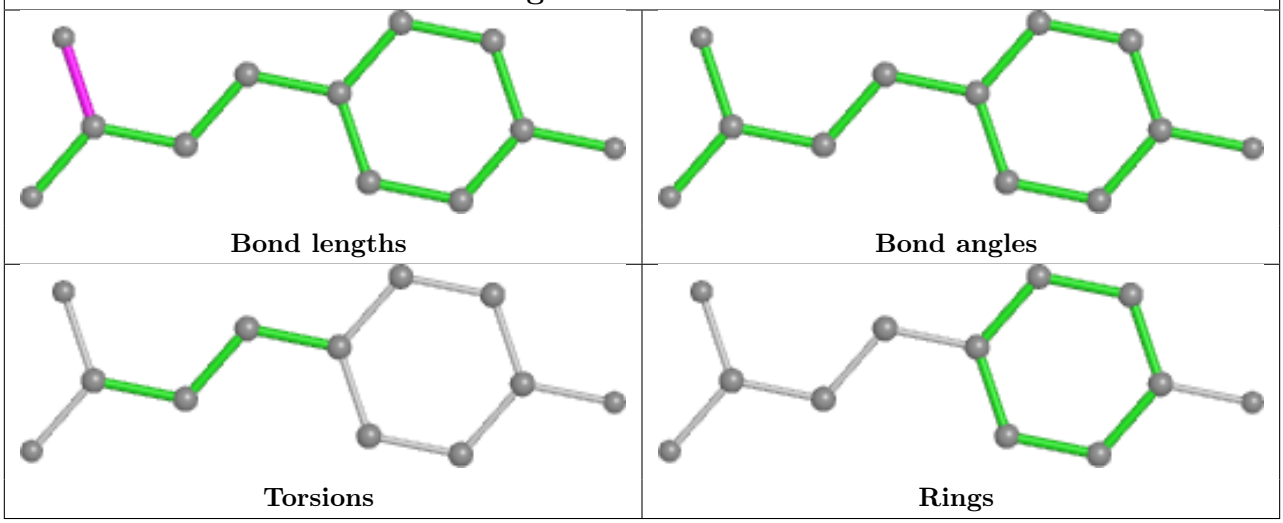
There are no ring outliers.

7 monomers are involved in 34 short contacts:

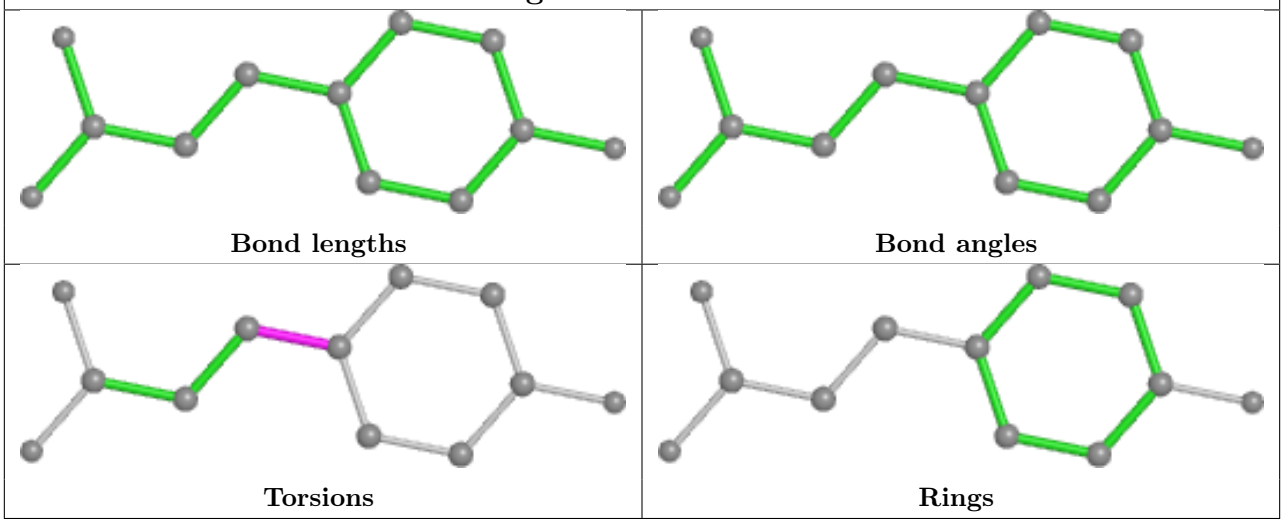
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	EDO	1	0
6	B	607	EDO	1	0
4	B	604	HC4	3	0
6	A	605	EDO	8	0
8	B	601	PG4	13	0
4	A	601	HC4	1	0
9	B	602	P6G	9	0

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.

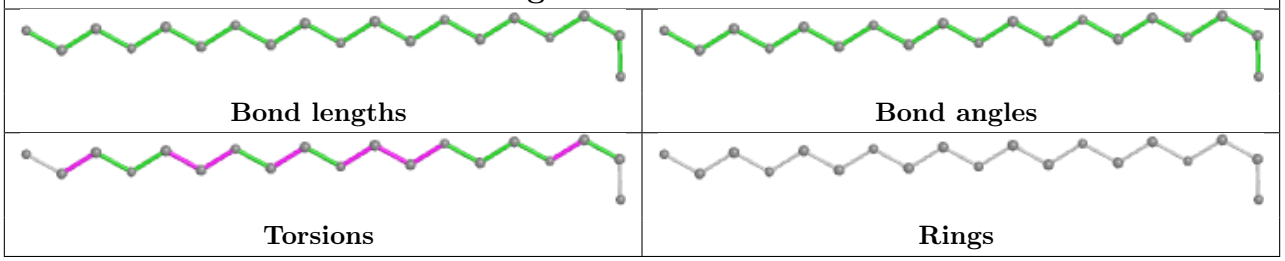
Ligand HC4 B 604



Ligand HC4 A 601



Ligand P6G B 602



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, 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	503/508 (99%)	-0.12	9 (1%) 68 72	18, 30, 57, 77	0
1	B	504/508 (99%)	-0.34	2 (0%) 92 93	16, 24, 38, 74	0
All	All	1007/1016 (99%)	-0.23	11 (1%) 80 83	16, 27, 52, 77	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	LEU	4.2
1	A	41	CYS	4.1
1	A	298	LYS	3.0
1	B	303	ASN	2.8
1	A	187	PHE	2.6
1	A	42	ALA	2.6
1	A	44	PHE	2.6
1	A	502	ASN	2.4
1	A	479	LEU	2.3
1	B	543	GLU	2.0
1	A	299	GLY	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

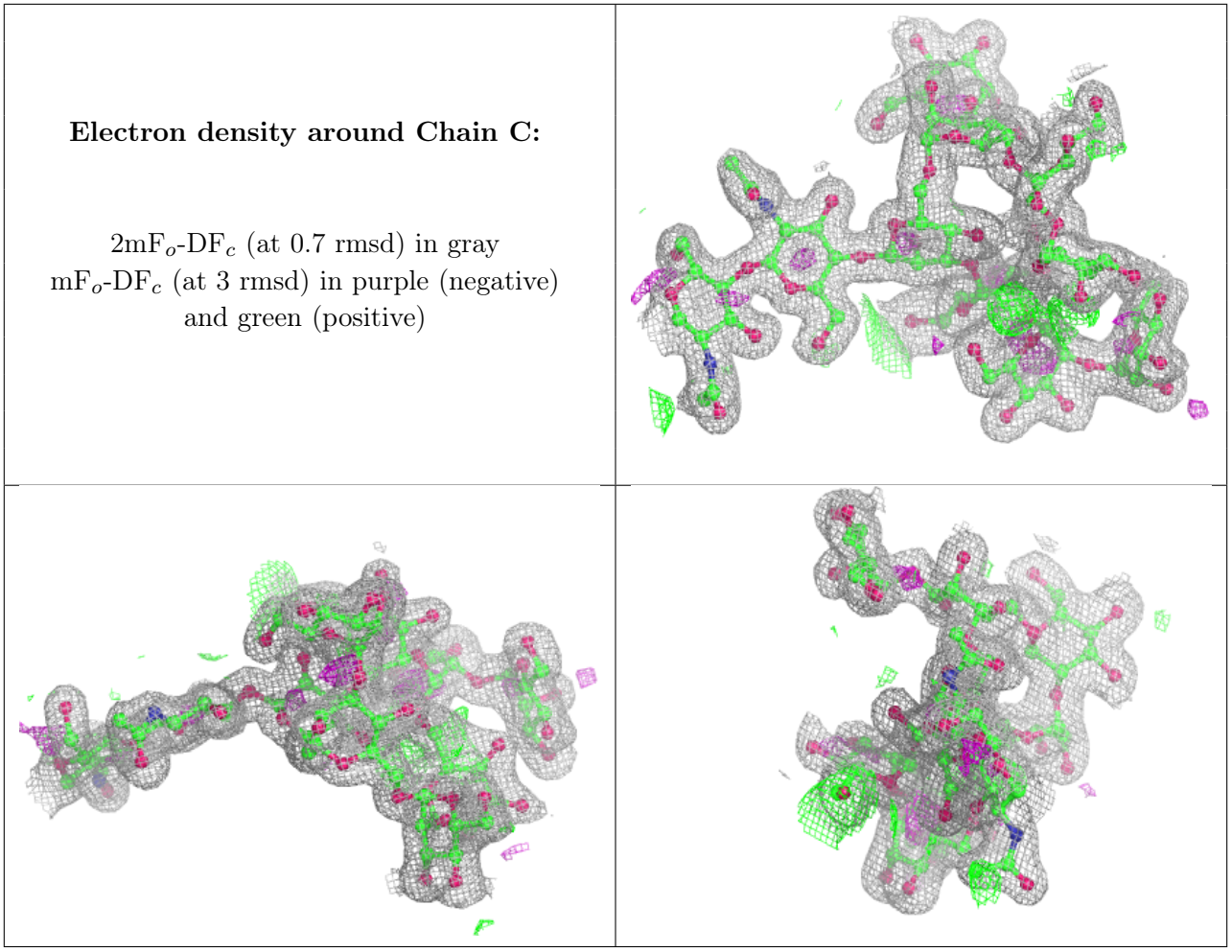
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MAN	G	9	11/12	0.81	0.19	48,56,60,69	0
3	MAN	E	4	11/12	0.83	0.22	43,54,57,57	0
3	BMA	E	3	11/12	0.86	0.22	41,58,69,77	0
2	MAN	G	10	11/12	0.87	0.10	34,37,41,42	0
2	MAN	C	4	11/12	0.88	0.12	28,31,37,46	0
2	MAN	C	9	11/12	0.89	0.12	39,45,60,61	0
3	MAN	E	5	11/12	0.89	0.12	40,44,49,49	0
2	MAN	C	5	11/12	0.90	0.10	29,33,37,42	0
3	MAN	E	6	11/12	0.90	0.17	36,40,42,57	0
2	MAN	I	4	11/12	0.91	0.08	20,22,29,38	0
3	NAG	E	1	14/15	0.91	0.09	37,41,50,54	0
2	MAN	G	7	11/12	0.91	0.08	31,34,37,38	0
3	NAG	E	2	14/15	0.92	0.09	40,46,53,58	0
2	MAN	C	8	11/12	0.94	0.06	23,26,31,31	0
2	MAN	C	6	11/12	0.94	0.10	38,40,44,44	0
2	MAN	I	10	11/12	0.94	0.10	29,32,40,56	0
2	NAG	C	1	14/15	0.95	0.09	24,27,33,43	0
2	NAG	C	2	14/15	0.95	0.07	25,28,35,35	0
2	NAG	I	2	14/15	0.95	0.07	25,27,30,31	0
2	BMA	C	3	11/12	0.95	0.07	21,23,24,25	0
2	MAN	I	5	11/12	0.95	0.09	24,25,36,41	0
2	MAN	G	8	11/12	0.95	0.08	30,32,38,43	0
2	MAN	I	9	11/12	0.96	0.07	23,25,26,26	0
2	NAG	I	1	14/15	0.96	0.08	23,26,31,32	0
2	BMA	G	3	11/12	0.96	0.07	22,23,26,27	0
2	MAN	G	4	11/12	0.96	0.08	20,21,27,35	0
2	NAG	G	2	14/15	0.96	0.06	22,23,26,28	0
2	MAN	I	6	11/12	0.96	0.08	26,33,39,40	0
2	MAN	I	7	11/12	0.96	0.07	20,22,25,27	0
2	MAN	I	8	11/12	0.96	0.08	21,23,28,32	0
2	MAN	G	6	11/12	0.97	0.06	18,21,22,23	0
2	NAG	G	1	14/15	0.97	0.06	25,27,34,37	0
2	MAN	C	7	11/12	0.97	0.09	21,23,25,25	0
2	MAN	G	5	11/12	0.97	0.07	21,22,24,24	0
2	BMA	I	3	11/12	0.98	0.07	19,21,23,23	0
2	MAN	C	10	11/12	0.98	0.07	22,27,29,30	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.

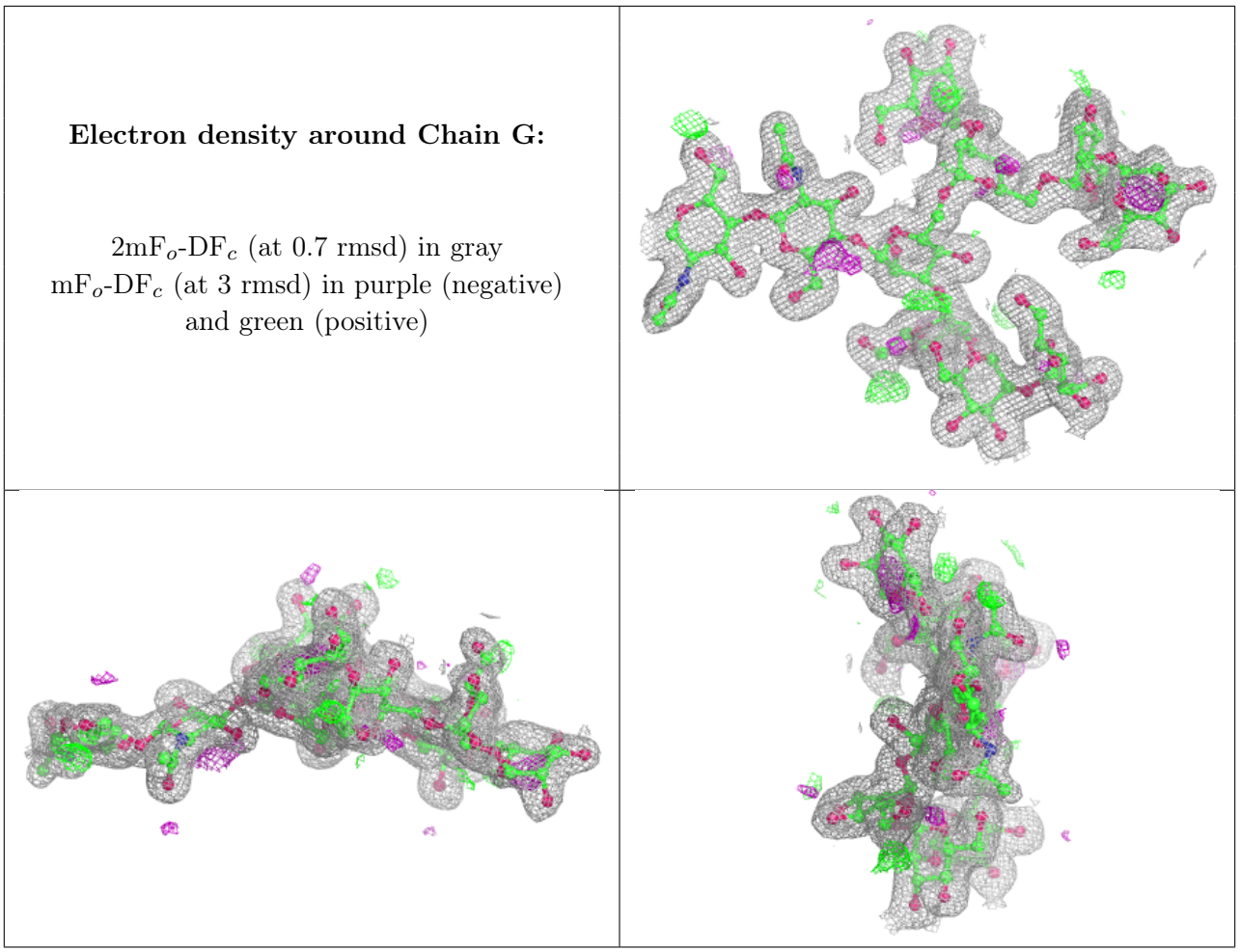
Electron density around Chain C:

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



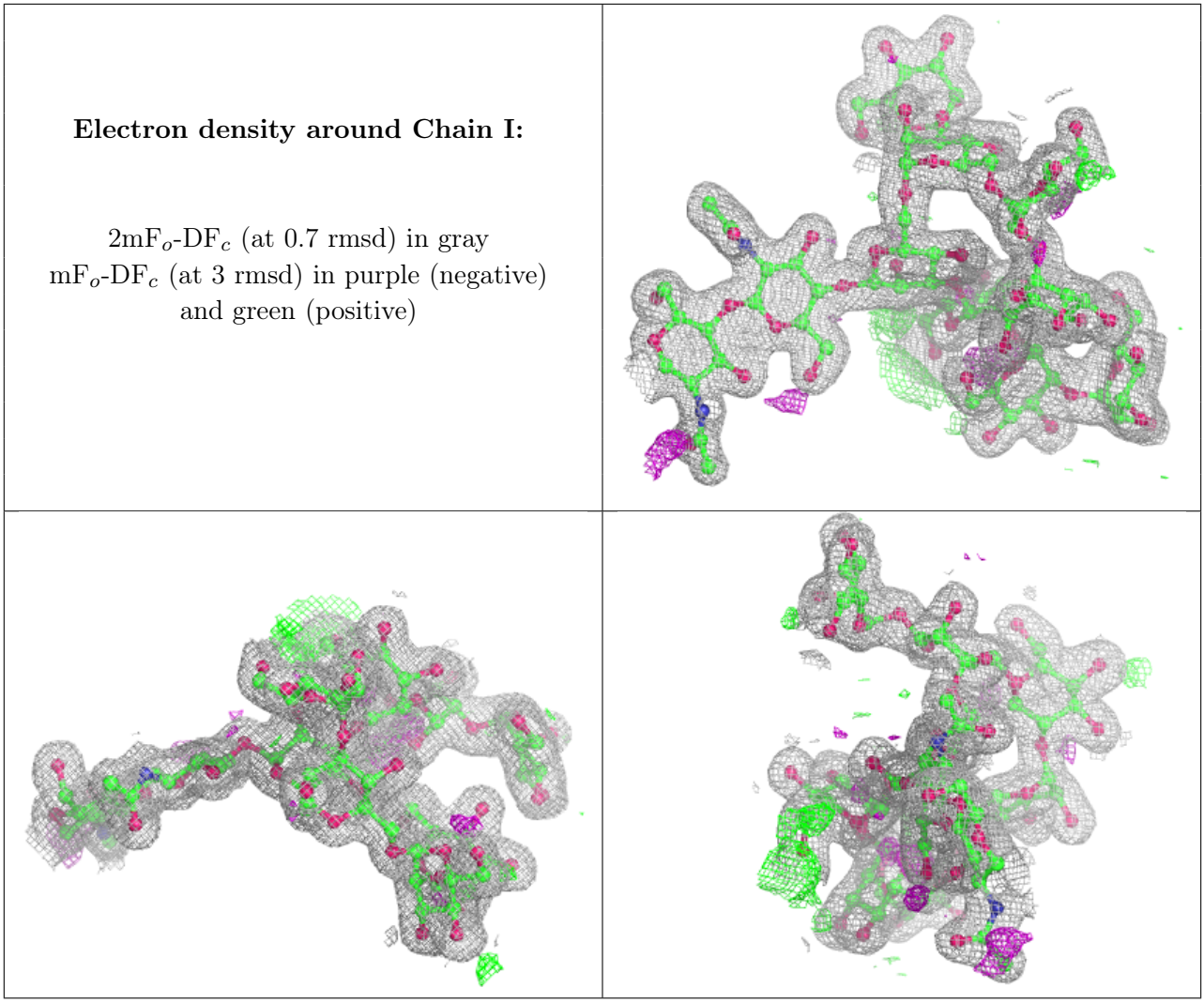
Electron density around Chain G:

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



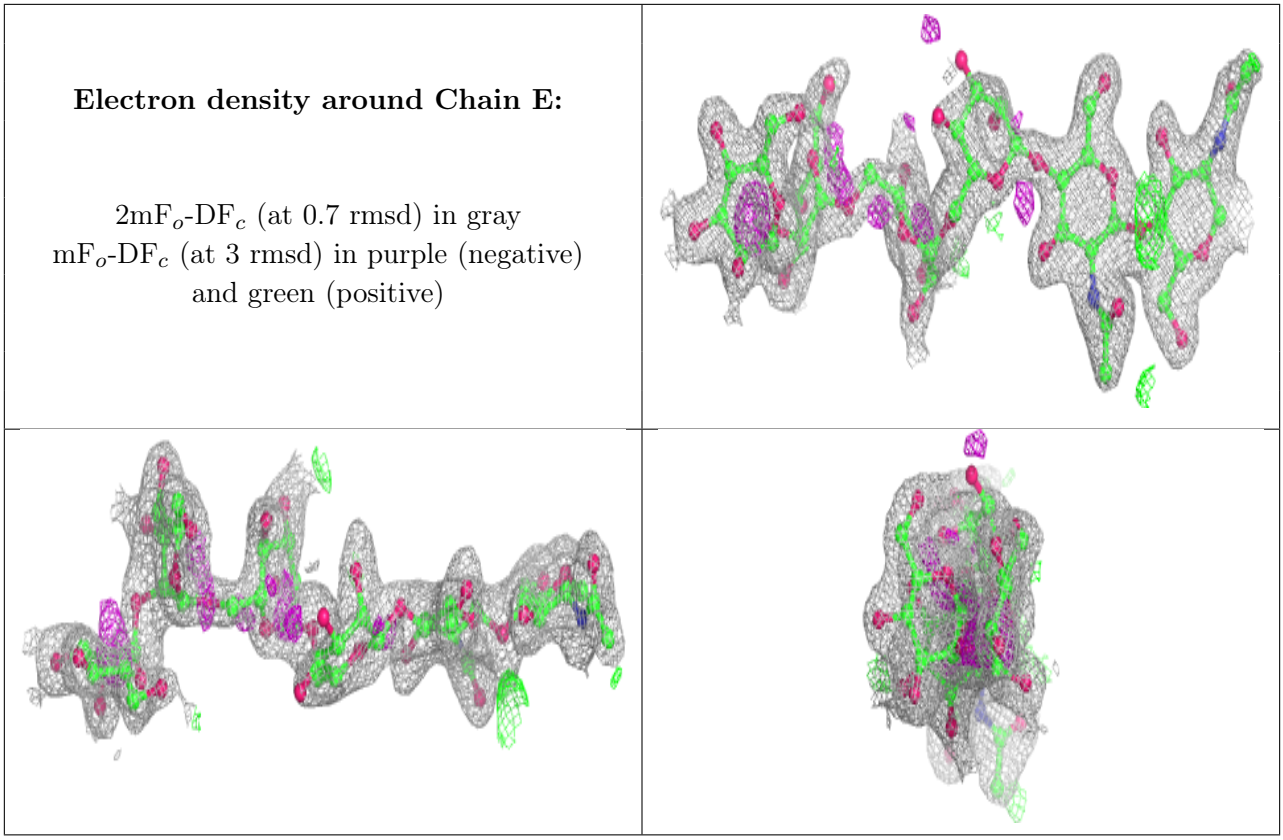
Electron density around Chain I:

$2mF_o$-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:

$2mF_o$-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	EDO	B	608	4/4	0.75	0.17	52,53,57,58	0
6	EDO	A	604	4/4	0.82	0.14	58,62,65,68	0
6	EDO	A	603	4/4	0.82	0.13	49,54,55,55	0
8	PG4	B	601	13/13	0.82	0.15	32,48,53,59	0
9	P6G	B	602	19/19	0.82	0.17	36,55,80,82	0
5	NAG	B	612	14/15	0.84	0.17	51,63,77,85	0
5	NAG	B	611	14/15	0.85	0.10	43,50,57,57	0
6	EDO	B	613	4/4	0.86	0.19	53,54,57,62	0
5	NAG	A	602	14/15	0.87	0.19	40,49,55,58	0
6	EDO	B	607	4/4	0.88	0.11	44,45,47,47	0
6	EDO	A	605	4/4	0.89	0.28	41,42,45,46	0
10	PEG	B	609	7/7	0.89	0.12	51,53,55,61	0
6	EDO	B	605	4/4	0.91	0.23	43,61,62,63	0
5	NAG	B	603	14/15	0.92	0.09	26,34,39,42	0

Continued on next page...

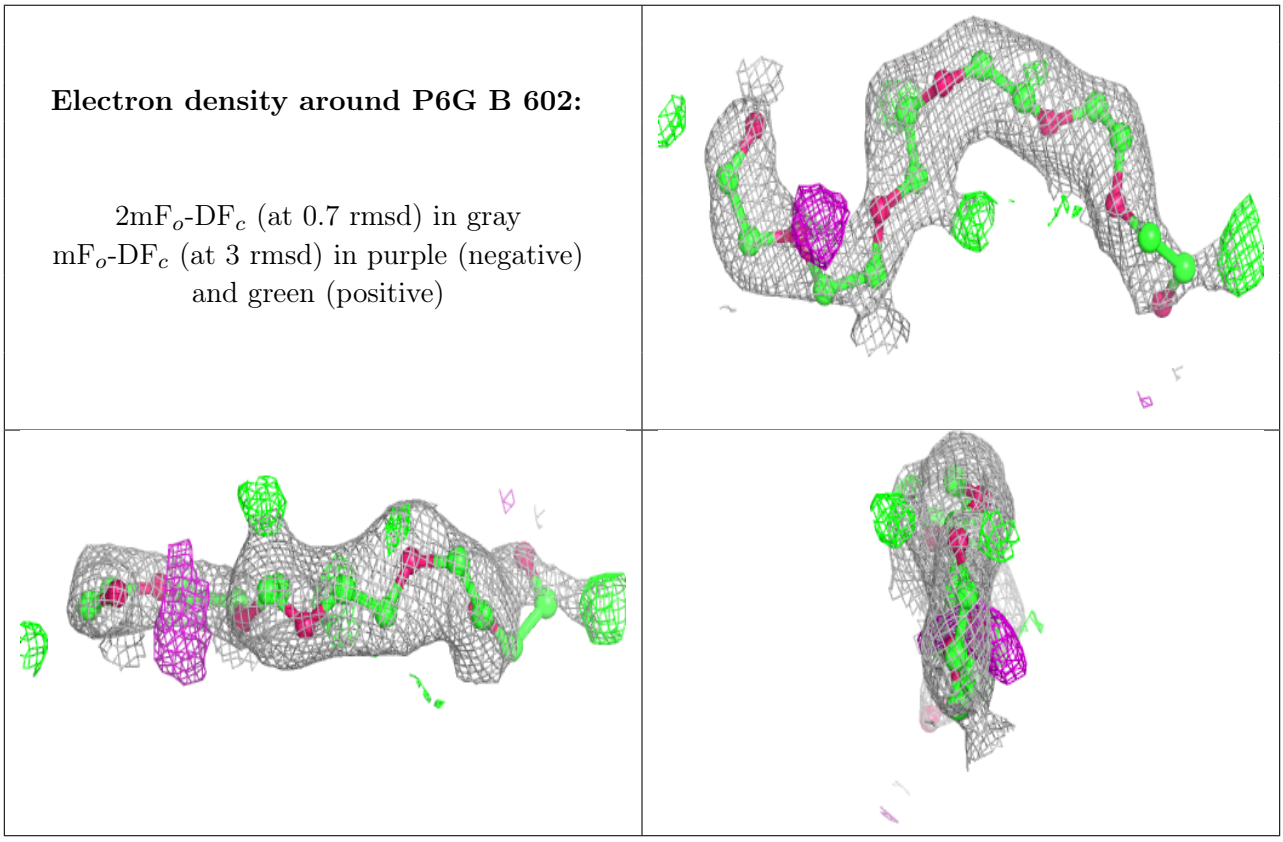
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	606	4/4	0.92	0.17	40,43,53,61	0
6	EDO	A	606	4/4	0.93	0.23	39,51,54,59	0
6	EDO	B	610	4/4	0.93	0.13	58,60,61,62	0
4	HC4	B	604	12/12	0.95	0.07	20,21,26,27	0
4	HC4	A	601	12/12	0.96	0.07	22,24,29,33	0
7	CA	B	614	1/1	1.00	0.07	26,26,26,26	0
7	CA	A	607	1/1	1.00	0.06	26,26,26,26	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.

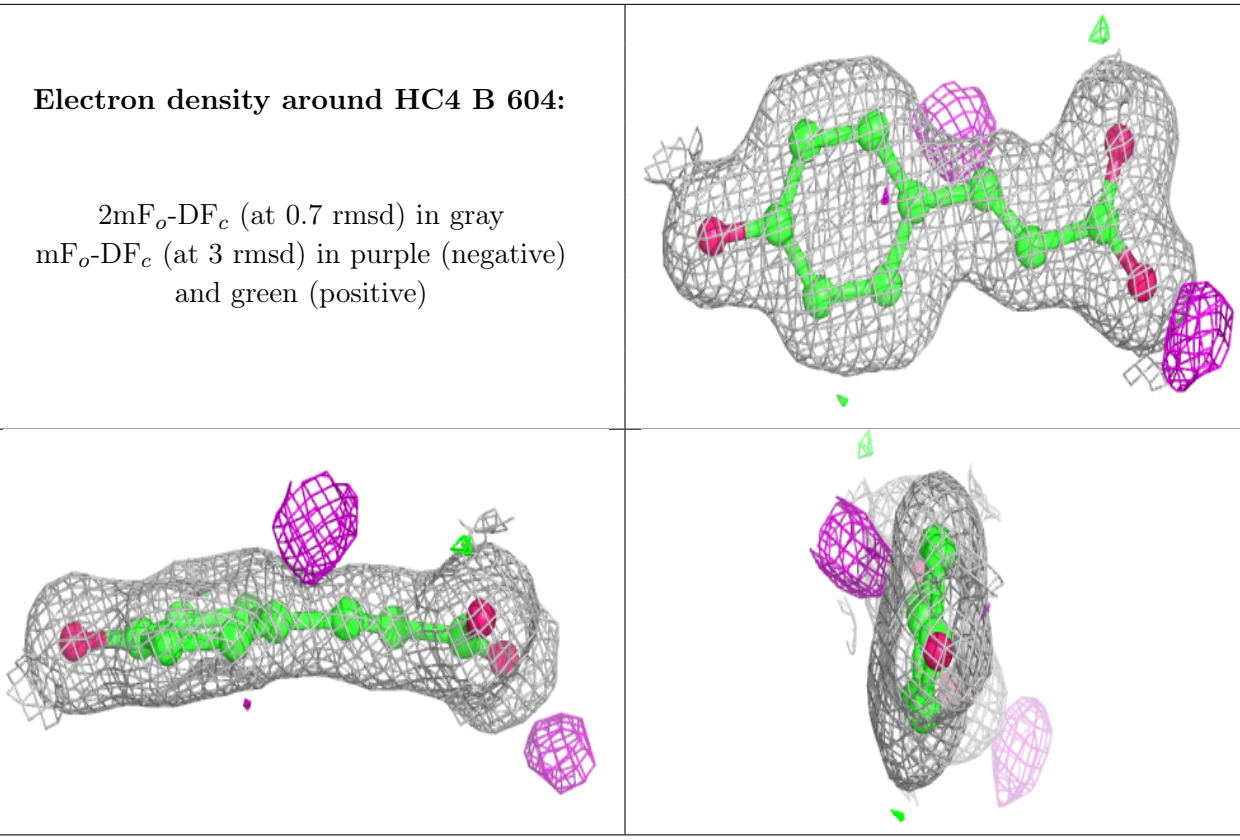
Electron density around P6G B 602:

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



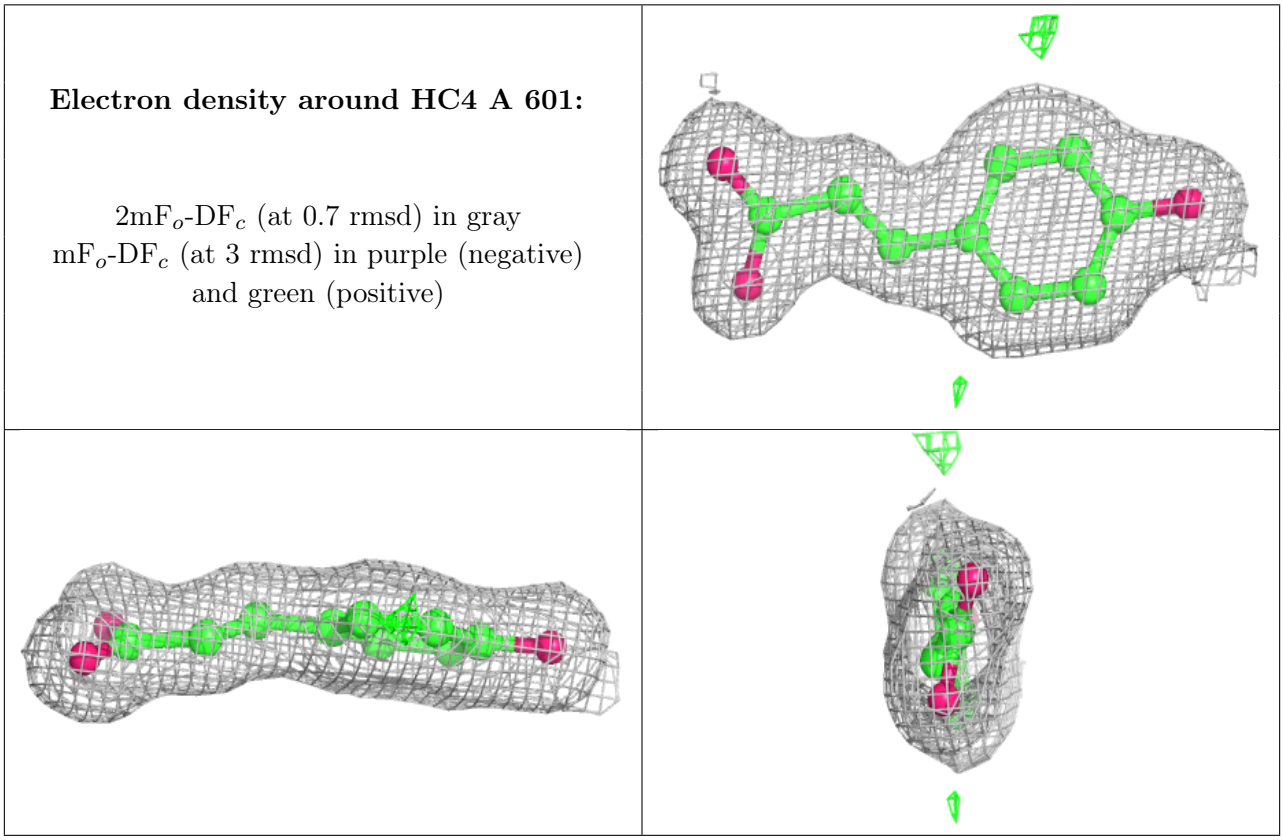
Electron density around HC4 B 604:

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



Electron density around HC4 A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.