Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:09 AM BST

PDB ID	:	6IC7
Title	:	Human cathepsin-C in complex with dipeptidyl cyclopropyl nitrile inhibitor 3
Authors	:	Hakansson, M.; Logan, D.T.; Korkmaz, B.; Lesner, A.; Wysocka, M.; Gieldon, A.; Gauthier, F.; Jenne, D.; Lauritzen, C.; Pedersen, J.
Deposited on	:	2018-12-02
Resolution	:	2.00 Å(reported)

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	119	10% 76% 20%
2	B	162	2% 88% 10%
3	C	69	3% 87% 12%
4	D	5	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3299 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 Dipeptidyl peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	976	628	156	185	7	0	5	0

- Molecule 2 is a protein called Dipeptidyl peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	162	1312	836	219	244	13	0	4	0

- Molecule 3 is a protein called Dipeptidyl peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	68	535	344	89	100	2	0	1	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
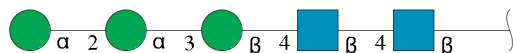
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	5	61	34	2	25	0	0	0

- 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	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1-azanyl- {N}-[(1 {R},2 {R})-1-cyano-2-[4-[4-(4-methylpiperazin-1-yl)sulfony lphenyl]phenyl]cyclopropyl]cyclohexane-1-carboxamide (three-letter code: H9H) (formula: $C_{28}H_{35}N_5O_3S$) (labeled as "Ligand of Interest" by author).

H9H
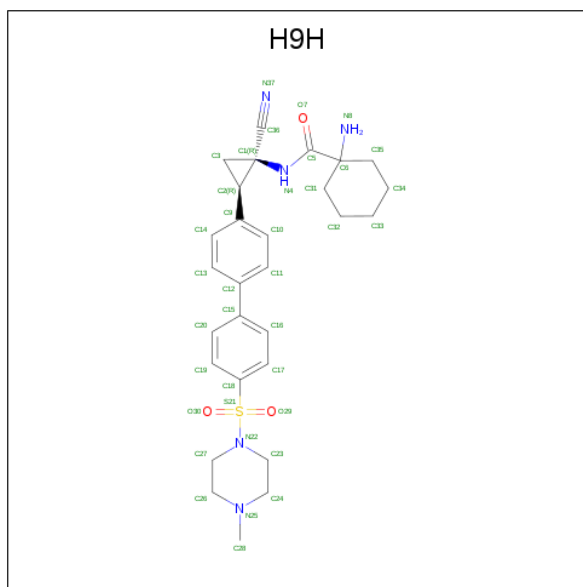
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	B	1	37	28	5	3	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total	O	0	0
			109	109		
8	B	174	Total	O	0	1
			174	174		
8	C	66	Total	O	0	0
			66	66		

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.
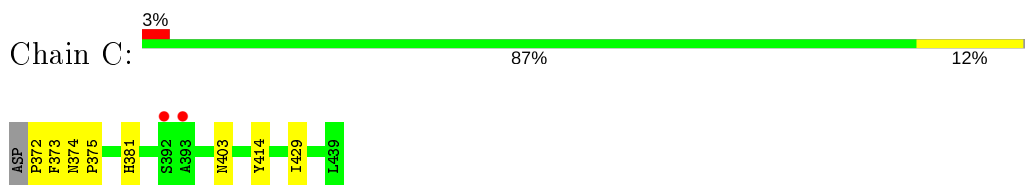
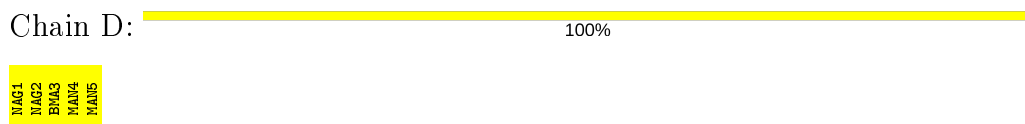- Molecule 1: Dipeptidyl peptidase 1
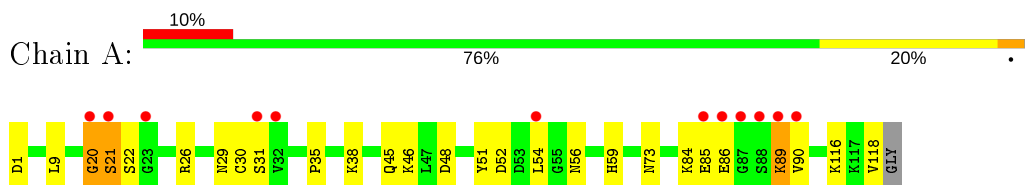
- Molecule 2: Dipeptidyl peptidase 1
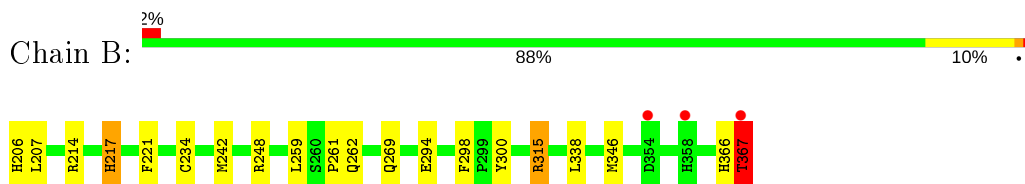
- Molecule 3: Dipeptidyl peptidase 1

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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.36Å 87.55Å 115.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.23 – 2.00 28.23 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.23-2.00) 83.5 (28.23-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.77 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0238 2018/15/10	Depositor
R, R_{free}	0.160 , 0.203 0.171 , 0.212	Depositor DCC
R_{free} test set	1757 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.2	EDS
L-test for twinning[2]	$<|L|> = 0.53, <L^2> = 0.37$	Xtriage
Estimated twinning fraction	0.001 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3299	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: H9H, MAN, BMA, NAG, CL

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	0.95	2/1011 (0.2%)	1.02	1/1372 (0.1%)
2	B	0.88	1/1359 (0.1%)	0.93	3/1842 (0.2%)
3	C	0.71	0/552	0.85	0/751
All	All	0.88	3/2922 (0.1%)	0.95	4/3965 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	294	GLU	CD-OE1	-9.12	1.15	1.25
1	A	20	GLY	C-O	7.95	1.36	1.23
1	A	21	SER	C-O	-5.09	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	315	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	30	CYS	CB-CA-C	6.53	123.45	110.40
2	B	367	THR	CA-C-O	-5.61	108.33	120.10
2	B	217	HIS	CB-CA-C	5.15	120.70	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	375[A]	PRO	Peptide

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	976	0	926	17	0
2	B	1312	0	1214	19	0
3	C	535	0	508	6	0
4	D	61	0	52	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	B	1	0	0	0	0
7	B	37	0	0	5	0
8	A	109	0	0	9	3
8	B	174	0	0	6	2
8	C	66	0	0	3	1
All	All	3299	0	2726	41	3

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 7.

All (41) 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)
2:B:234:CYS:SG	7:B:403:H9H:C36	2.17	1.33
1:A:73[B]:ASN:ND2	8:A:701:HOH:O	1.88	1.06
1:A:31:SER:HA	8:A:729:HOH:O	1.64	0.96
1:A:52:ASP:OD2	1:A:73[A]:ASN:ND2	2.08	0.85
1:A:20:GLY:O	1:A:21:SER:HB2	1.77	0.82
2:B:234:CYS:SG	7:B:403:H9H:N37	2.51	0.82
1:A:73[B]:ASN:CG	8:A:701:HOH:O	2.15	0.75
1:A:86:GLU:O	1:A:89:LYS:HB3	1.97	0.64
1:A:54:LEU:N	8:A:703:HOH:O	2.30	0.64
2:B:269[B]:GLN:NE2	8:B:502:HOH:O	2.31	0.63
1:A:73[B]:ASN:ND2	8:A:704:HOH:O	2.31	0.63
1:A:45:GLN:NE2	1:A:51[B]:TYR:HE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269[B]:GLN:HG2	8:B:501:HOH:O	2.02	0.59
1:A:9:LEU:HG	8:A:792:HOH:O	2.02	0.59
1:A:29:ASN:ND2	8:A:706:HOH:O	2.32	0.58
2:B:217:HIS:HD2	8:B:646:HOH:O	1.88	0.56
1:A:85:GLU:HG3	1:A:90:VAL:HG22	1.86	0.56
2:B:234:CYS:SG	7:B:403:H9H:C1	2.92	0.55
2:B:269[B]:GLN:NE2	8:B:501:HOH:O	2.27	0.55
2:B:366:HIS:O	2:B:367:THR:HB	2.06	0.54
2:B:259:LEU:O	2:B:261:PRO:HD3	2.12	0.50
1:A:85:GLU:CG	1:A:90:VAL:HG22	2.42	0.49
1:A:48:ASP:O	1:A:59:HIS:HA	2.15	0.47
2:B:248[A]:ARG:NH2	8:B:508:HOH:O	2.49	0.46
3:C:373:PHE:HA	8:C:519:HOH:O	2.16	0.45
2:B:234:CYS:CB	7:B:403:H9H:N37	2.80	0.45
3:C:381:HIS:HE1	3:C:403:ASN:OD1	1.98	0.45
2:B:262:GLN:HB2	2:B:300:TYR:HA	1.99	0.45
1:A:73[A]:ASN:HB3	8:A:701:HOH:O	2.18	0.44
2:B:315:ARG:HD2	8:B:606:HOH:O	2.18	0.44
3:C:374:ASN:OD1	3:C:374:ASN:C	2.55	0.44
2:B:214:ARG:HD3	3:C:414:TYR:CZ	2.53	0.43
2:B:234:CYS:SG	7:B:403:H9H:N4	2.92	0.43
3:C:372:PRO:N	8:C:504:HOH:O	2.52	0.42
2:B:242:MET:SD	2:B:346:MET:HA	2.59	0.42
1:A:116:LYS:HE2	8:A:748:HOH:O	2.20	0.41
3:C:381:HIS:CD2	8:C:550:HOH:O	2.73	0.41
2:B:207:LEU:HD11	2:B:338:LEU:HD23	2.03	0.41
2:B:221:PHE:O	2:B:248[B]:ARG:HD3	2.20	0.41
2:B:367:THR:O	2:B:367:THR:HG22	2.22	0.40
1:A:54:LEU:HB3	1:A:56:ASN:HD21	1.86	0.40

All (3) 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)
8:A:794:HOH:O	8:B:605:HOH:O[3_555]	1.71	0.49
8:A:801:HOH:O	8:B:622:HOH:O[8_444]	2.12	0.08
8:A:796:HOH:O	8:C:561:HOH:O[2_545]	2.14	0.06

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	121/119 (102%)	114 (94%)	7 (6%)	0	100	100
2	B	164/162 (101%)	158 (96%)	6 (4%)	0	100	100
3	C	67/69 (97%)	59 (88%)	7 (10%)	1 (2%)	10	4
All	All	352/350 (101%)	331 (94%)	20 (6%)	1 (0%)	41	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	429	ILE

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	108/103 (105%)	99 (92%)	9 (8%)	11	7
2	B	141/137 (103%)	138 (98%)	3 (2%)	53	57
3	C	55/55 (100%)	55 (100%)	0	100	100
All	All	304/295 (103%)	292 (96%)	12 (4%)	30	30

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

Mol	Chain	Res	Type
1	A	1	ASP
1	A	22	SER

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Mol	Chain	Res	Type
1	A	26	ARG
1	A	35	PRO
1	A	38	LYS
1	A	46	LYS
1	A	84	LYS
1	A	89	LYS
1	A	118	VAL
2	B	206	HIS
2	B	298	PHE
2	B	367	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	56	ASN
3	C	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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
4	NAG	D	1	1,4	14,14,15	0.80	0	17,19,21	2.31	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	D	2	4	14,14,15	0.74	0	17,19,21	1.41	2 (11%)
4	BMA	D	3	4	11,11,12	0.61	0	15,15,17	1.04	1 (6%)
4	MAN	D	4	4	11,11,12	0.79	0	15,15,17	1.58	3 (20%)
4	MAN	D	5	4	11,11,12	1.07	1 (9%)	15,15,17	1.36	3 (20%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	MAN	O5-C1	2.44	1.47	1.43

All (14) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	C1-O5-C5	-5.21	105.14	112.19
4	D	1	NAG	O6-C6-C5	-5.08	93.85	111.29
4	D	4	MAN	C1-O5-C5	3.90	117.47	112.19
4	D	1	NAG	C3-C4-C5	-3.30	104.36	110.24
4	D	2	NAG	O5-C5-C6	3.04	111.98	107.20
4	D	4	MAN	O5-C5-C6	3.04	111.97	107.20
4	D	2	NAG	C1-O5-C5	-3.00	108.13	112.19
4	D	1	NAG	O4-C4-C3	-2.68	104.14	110.35
4	D	5	MAN	C1-O5-C5	2.68	115.83	112.19
4	D	4	MAN	C1-C2-C3	-2.58	106.50	109.67
4	D	3	BMA	C1-O5-C5	2.43	115.49	112.19
4	D	5	MAN	O4-C4-C3	2.27	115.59	110.35
4	D	1	NAG	C2-N2-C7	-2.22	119.74	122.90
4	D	5	MAN	O6-C6-C5	-2.02	104.35	111.29

There are no chirality outliers.

There are no torsion outliers.

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.
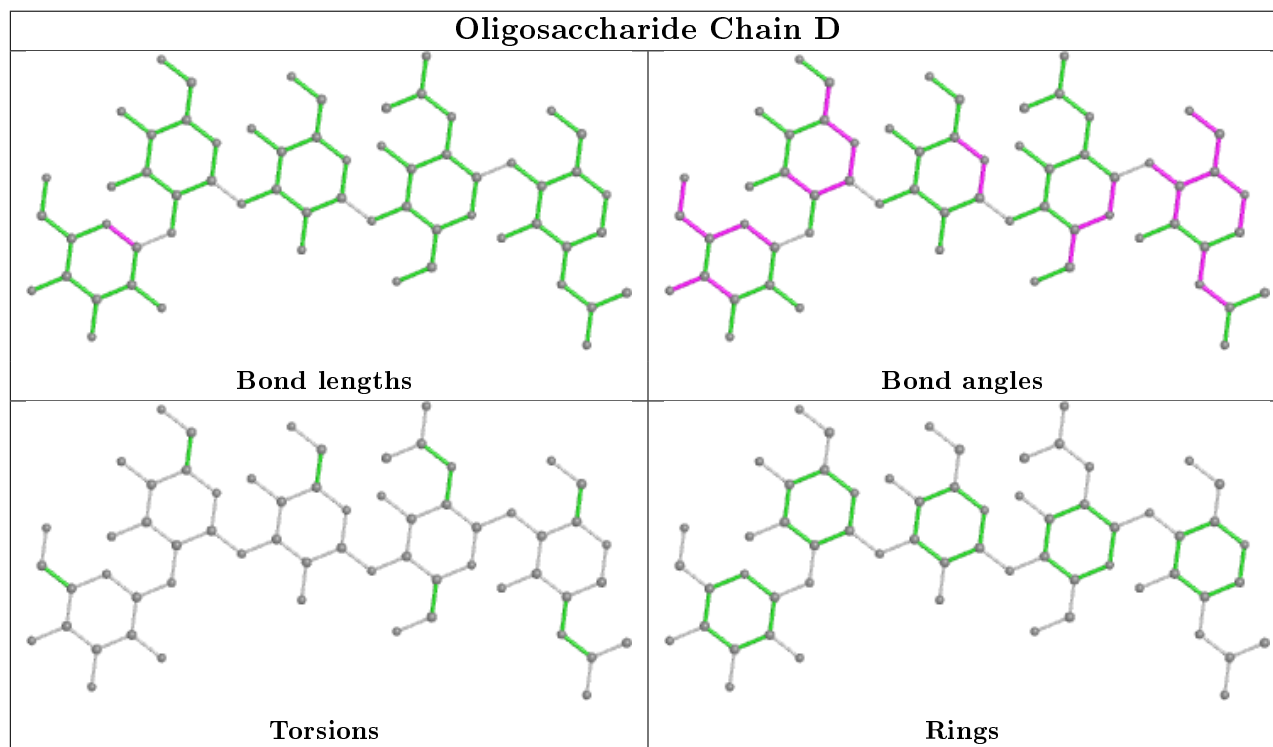
5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	#$|Z| > 2$
5	NAG	B	401	2	14,14,15	0.76	0	17,19,21	1.30	1 (5%)
5	NAG	A	601	1	14,14,15	1.11	0	17,19,21	3.26	6 (35%)
7	H9H	B	403	-	37,41,41	1.94	7 (18%)	48,62,62	1.92	13 (27%)

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
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1	-	3/6/23/26	0/1/1/1
7	H9H	B	403	-	-	5/28/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	H9H	S21-N22	7.06	1.73	1.63
7	B	403	H9H	C1-C36	-4.04	1.43	1.48
7	B	403	H9H	O29-S21	3.67	1.47	1.43
7	B	403	H9H	O30-S21	3.29	1.47	1.43
7	B	403	H9H	C19-C18	2.16	1.42	1.38
7	B	403	H9H	C13-C12	2.14	1.43	1.39
7	B	403	H9H	C5-N4	2.05	1.37	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	NAG	C2-N2-C7	7.83	134.06	122.90
5	A	601	NAG	C1-C2-N2	5.85	120.49	110.49
5	A	601	NAG	O7-C7-N2	5.15	131.41	121.95
7	B	403	H9H	C18-S21-N22	-5.02	101.32	107.30
5	A	601	NAG	C8-C7-N2	-4.91	107.78	116.10
7	B	403	H9H	O30-S21-O29	4.84	127.37	119.52
7	B	403	H9H	C24-C23-N22	4.56	112.40	108.91
7	B	403	H9H	C23-N22-C27	4.55	117.20	112.17
5	A	601	NAG	O4-C4-C3	-4.33	100.35	110.35
7	B	403	H9H	C31-C6-C35	3.18	113.47	108.40
5	B	401	NAG	C1-C2-N2	-3.10	105.19	110.49
7	B	403	H9H	C2-C1-N4	2.75	124.02	117.46
7	B	403	H9H	O30-S21-N22	-2.72	104.21	106.69
5	A	601	NAG	O4-C4-C5	2.66	115.90	109.30
7	B	403	H9H	C28-N25-C24	2.66	114.64	110.66
7	B	403	H9H	C13-C14-C9	-2.36	118.82	121.20
7	B	403	H9H	O7-C5-C6	-2.31	116.55	120.36
7	B	403	H9H	C20-C19-C18	-2.20	117.17	119.45
7	B	403	H9H	C3-C2-C9	-2.15	120.06	123.45
7	B	403	H9H	C14-C9-C10	2.07	120.87	118.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	403	H9H	O7-C5-C6-C31
5	A	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C1-C2-N2-C7
7	B	403	H9H	N4-C5-C6-C31
7	B	403	H9H	C1-C2-C9-C10
7	B	403	H9H	C1-C2-C9-C14
7	B	403	H9H	C27-N22-S21-O29

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	403	H9H	5	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 H9H B 403

Bond lengths

Bond angles

Torsions

Rings
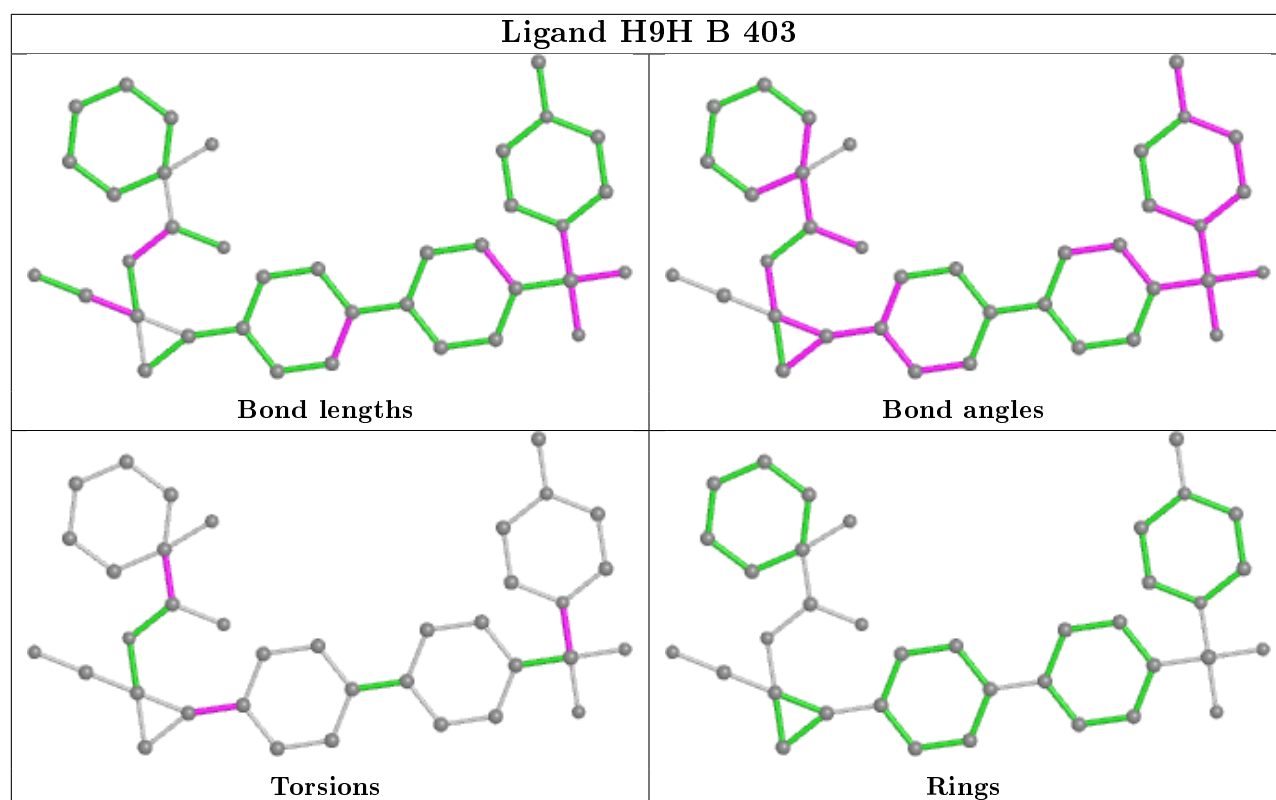
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	118/119 (99%)	0.05	12 (10%)	6	6	10, 18, 45, 80	1 (0%)
2	B	162/162 (100%)	-0.40	3 (1%)	66	65	9, 15, 37, 51	0
3	C	68/69 (98%)	-0.24	2 (2%)	51	50	11, 18, 42, 52	0
All	All	348/350 (99%)	-0.21	17 (4%)	29	28	9, 17, 42, 80	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	SER	6.8
1	A	87	GLY	5.6
1	A	86	GLU	4.0
1	A	32	VAL	3.8
1	A	89	LYS	3.5
3	C	393	ALA	3.4
2	B	367	THR	3.4
1	A	85	GLU	3.0
1	A	31	SER	2.9
1	A	54	LEU	2.7
2	B	358	HIS	2.7
2	B	354[A]	ASP	2.6
1	A	21	SER	2.5
1	A	90	VAL	2.5
1	A	23	GLY	2.4
1	A	20	GLY	2.2
3	C	392	SER	2.2

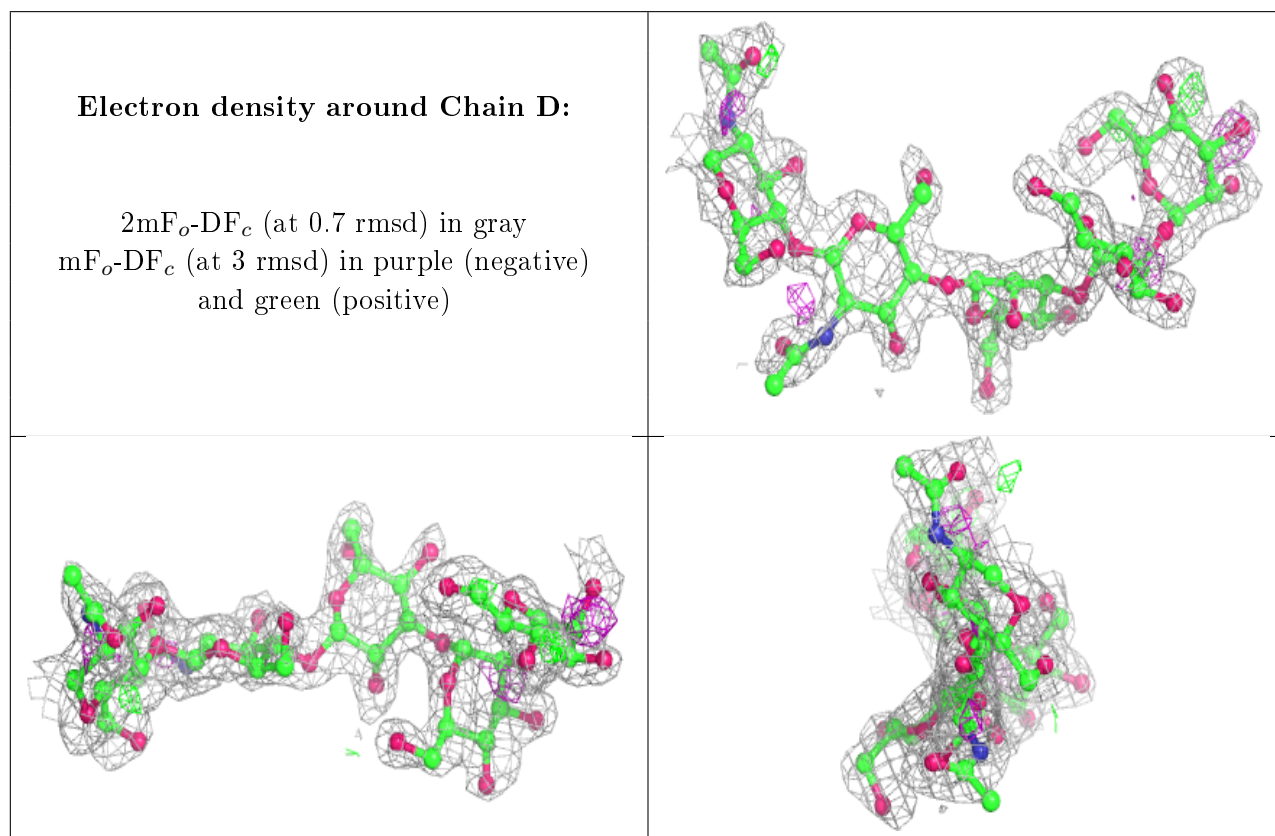## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	MAN	D	5	11/12	0.70	0.27	41,47,54,54	0
4	NAG	D	1	14/15	0.83	0.25	35,40,43,45	0
4	MAN	D	4	11/12	0.83	0.30	45,51,55,55	0
4	BMA	D	3	11/12	0.84	0.29	49,51,53,57	0
4	NAG	D	2	14/15	0.85	0.29	41,45,49,50	0

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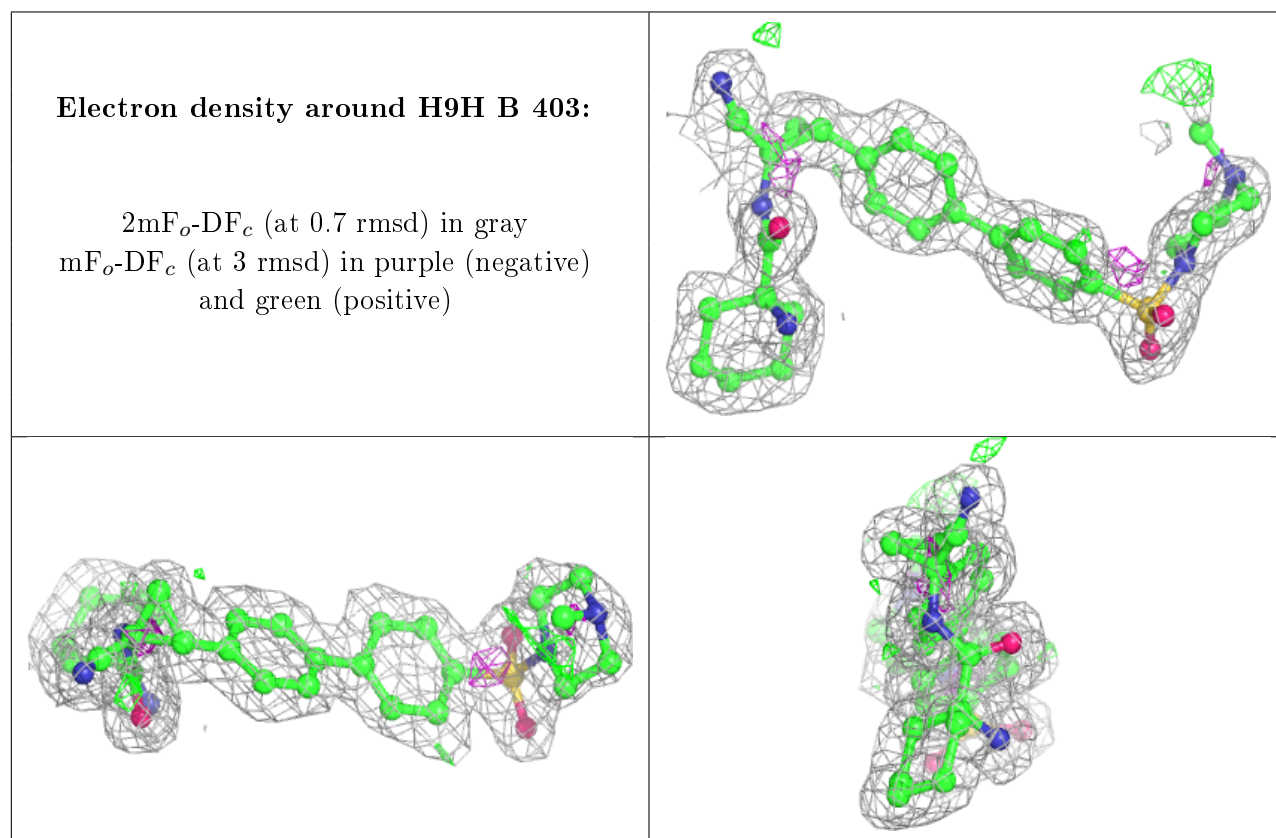

Electron density around Chain D:

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

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	601	14/15	0.75	0.33	41,51,55,57	0
5	NAG	B	401	14/15	0.81	0.26	32,38,43,46	0
7	H9H	B	403	37/37	0.90	0.14	14,20,43,49	0
6	CL	B	402	1/1	1.00	0.07	13,13,13,13	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 H9H B 403:

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

6.5   Other polymers (i)

There are no such residues in this entry.