Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 07:28 AM EDT

PDB ID	:	2RIP
Title	:	Structure of DPPIV in complex with an inhibitor
Authors	:	Qiu, X.
Deposited on	:	2007-10-12
Resolution	:	2.90 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:

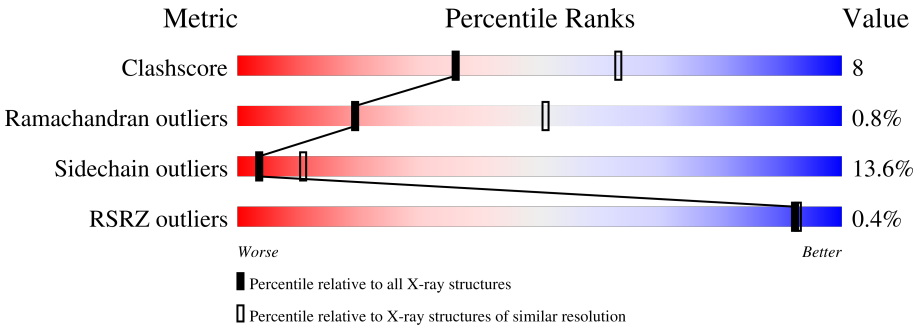
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	729	70% 27% .
2	B	4	50% 50%
3	C	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
2	NAG	B	2	X	-	-	-
2	MAN	B	3	X	-	-	-
2	MAN	B	4	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6158 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.

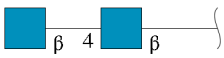
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	729	5972	3831	983	1132	26	0	0	0

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

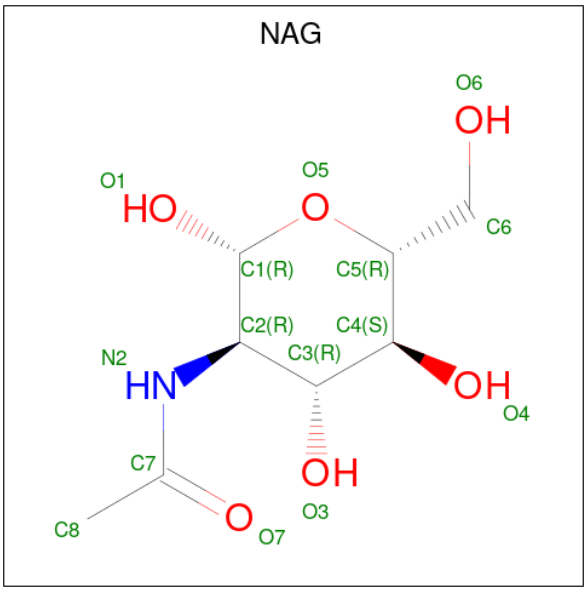
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

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



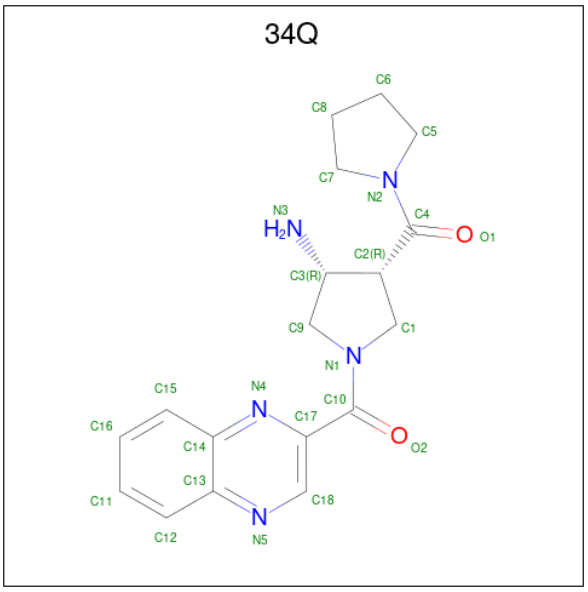
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is (3R,4R)-4-(pyrrolidin-1-ylcarbonyl)-1-(quinoxalin-2-ylcarbonyl)pyrrolidin-3-amine (three-letter code: 34Q) (formula: $C_{18}H_{21}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 6 is water.

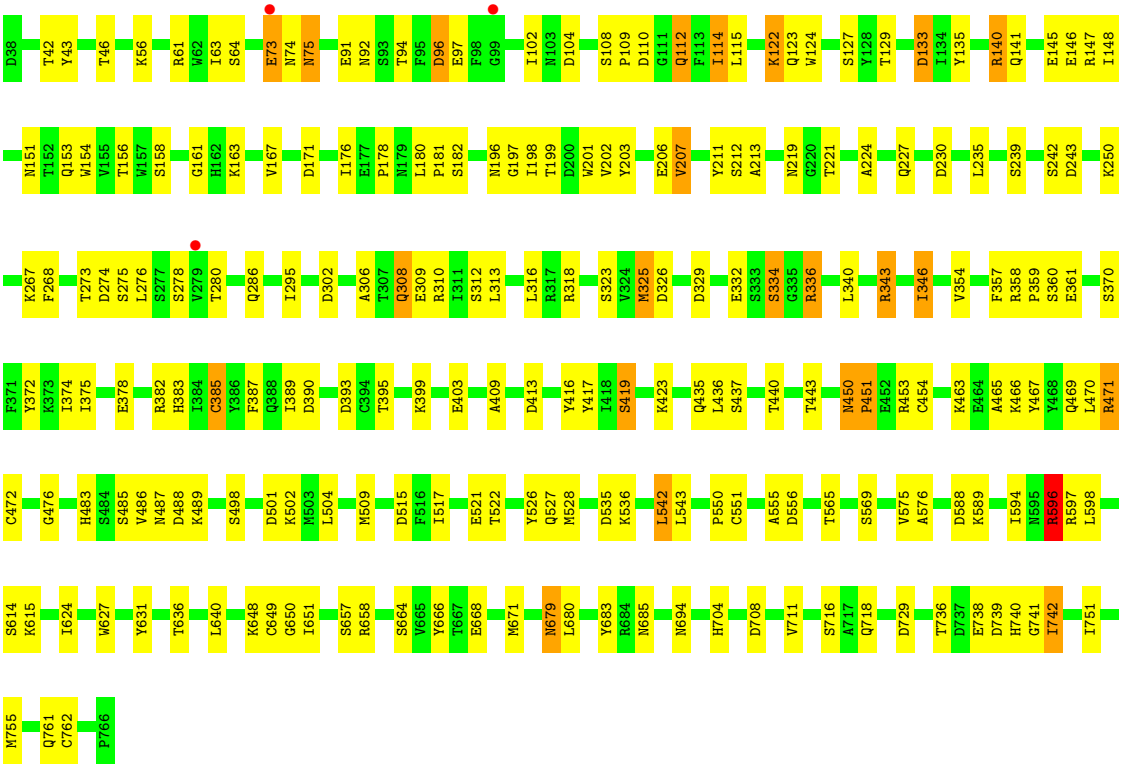
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		

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: Dipeptidyl peptidase 4

Chain A:



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

Chain B:

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

Chain C:


NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.22Å 69.22Å 409.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-2.90) 90.5 (48.95-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.293 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6158	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: MAN, 34Q, NAG

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	0.56	0/6144	0.81	19/8355 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	171	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	302	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	96	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	390	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	588	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	729	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	535	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	393	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	133	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	488	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	515	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	501	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	556	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	739	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	274	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	104	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	230	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	329	ASP	CB-CG-OD2	5.12	122.91	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	5972	0	5687	93	0
2	B	50	0	43	1	0
3	C	28	0	25	2	0
4	A	56	0	52	1	0
5	A	25	0	21	1	0
6	A	27	0	0	0	0
All	All	6158	0	5828	96	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 8.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HE21	1:A:308:GLN:HA	1.11	1.11
1:A:704:HIS:HD2	1:A:716:SER:OG	1.38	1.06
1:A:308:GLN:HA	1:A:308:GLN:NE2	1.68	1.02
1:A:648:LYS:HE2	1:A:762:CYS:O	1.74	0.88
1:A:308:GLN:HE21	1:A:308:GLN:CA	1.88	0.86
1:A:704:HIS:CD2	1:A:716:SER:OG	2.28	0.85
1:A:542:LEU:HD23	1:A:624:ILE:HG23	1.63	0.79
1:A:334:SER:HB2	1:A:336:ARG:HG2	1.67	0.75
1:A:219:ASN:HB2	1:A:308:GLN:CD	2.09	0.73
1:A:146:GLU:HG2	1:A:181:PRO:HA	1.71	0.72
1:A:469:GLN:OE1	1:A:471:ARG:HD3	1.94	0.67
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.77	0.67
1:A:203:TYR:HA	1:A:207:VAL:HG23	1.78	0.65
1:A:153:GLN:HG2	1:A:211:TYR:OH	1.97	0.65
1:A:708:ASP:OD2	1:A:740:HIS:HA	1.98	0.64
1:A:334:SER:HB2	1:A:336:ARG:CG	2.28	0.63
1:A:74:ASN:C	1:A:92:ASN:HB3	2.19	0.62
1:A:122:LYS:HE2	1:A:124:TRP:O	2.01	0.61
1:A:308:GLN:NE2	1:A:308:GLN:CA	2.47	0.59
1:A:664:SER:HB2	1:A:668:GLU:OE2	2.03	0.58
3:C:1:NAG:H61	3:C:2:NAG:H83	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:THR:HG21	1:A:651:ILE:O	2.05	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:A:219:ASN:HB2	1:A:308:GLN:NE2	2.19	0.57
1:A:318:ARG:O	1:A:318:ARG:HG3	2.05	0.57
1:A:219:ASN:H	1:A:308:GLN:HE22	1.52	0.55
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.36	0.55
1:A:465:ALA:O	1:A:485:SER:OG	2.20	0.55
3:C:1:NAG:C6	3:C:2:NAG:H83	2.37	0.54
1:A:206:GLU:OE2	1:A:666:TYR:HB2	2.06	0.54
1:A:454:CYS:SG	1:A:472:CYS:SG	3.06	0.54
1:A:679:ASN:O	1:A:683:TYR:HD2	1.91	0.53
1:A:527:GLN:HG2	1:A:555:ALA:HA	1.91	0.53
1:A:221:THR:O	1:A:273:THR:OG1	2.27	0.53
1:A:680:LEU:HG	1:A:680:LEU:O	2.09	0.53
1:A:382:ARG:H	1:A:403:GLU:HG2	1.74	0.52
1:A:308:GLN:HB3	4:A:1219:NAG:H61	1.92	0.52
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.45	0.51
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.51
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.92	0.51
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.50
1:A:340:LEU:HB3	1:A:343:ARG:HG3	1.93	0.50
1:A:385:CYS:HB3	1:A:387:PHE:HE1	1.76	0.50
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.93	0.50
1:A:109:PRO:HG2	1:A:158:SER:O	2.12	0.49
1:A:140:ARG:O	1:A:140:ARG:CG	2.59	0.49
1:A:551:CYS:SG	1:A:551:CYS:O	2.71	0.49
1:A:454:CYS:HG	1:A:472:CYS:HG	1.58	0.49
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.49	0.48
1:A:199:THR:HB	1:A:203:TYR:HB3	1.94	0.48
1:A:550:PRO:HB3	1:A:594:ILE:HD11	1.96	0.47
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.47
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.96	0.47
1:A:167:VAL:HG21	1:A:198:ILE:HG23	1.95	0.47
1:A:372:TYR:HA	1:A:385:CYS:O	2.15	0.47
1:A:450:ASN:N	1:A:451:PRO:CD	2.78	0.46
1:A:409:ALA:HB3	1:A:416:TYR:HB2	1.98	0.46
1:A:374:ILE:O	1:A:375:ILE:HD12	2.16	0.46
1:A:738:GLU:HG3	1:A:742:ILE:HG23	1.97	0.46
1:A:374:ILE:HA	1:A:383:HIS:O	2.16	0.45
2:B:1:NAG:H61	2:B:2:NAG:HN2	1.81	0.45
1:A:64:SER:O	1:A:463:LYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:O	1:A:140:ARG:HG2	2.15	0.45
1:A:417:TYR:CE1	1:A:419:SER:HB3	2.52	0.45
1:A:123:GLN:HB3	1:A:127:SER:OG	2.16	0.45
1:A:110:ASP:OD1	1:A:112:GLN:HB2	2.17	0.45
1:A:109:PRO:HD2	1:A:161:GLY:O	2.16	0.45
1:A:528:MET:HG2	1:A:576:ALA:HB2	1.99	0.44
1:A:649:CYS:HG	1:A:762:CYS:CB	2.30	0.44
1:A:346:ILE:HG22	1:A:346:ILE:O	2.18	0.44
1:A:417:TYR:HE1	1:A:419:SER:HB3	1.83	0.44
1:A:354:VAL:HG12	1:A:359:PRO:HG3	1.99	0.43
1:A:704:HIS:HE1	1:A:711:VAL:O	2.00	0.43
1:A:751:ILE:O	1:A:755:MET:HG3	2.18	0.43
1:A:75:ASN:HB3	1:A:91:GLU:HA	2.00	0.43
1:A:504:LEU:HD22	1:A:509:MET:SD	2.58	0.43
1:A:123:GLN:HB3	1:A:124:TRP:H	1.70	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:A:201:TRP:CE3	1:A:202:VAL:HA	2.54	0.43
1:A:316:LEU:HD13	1:A:323:SER:HB2	2.00	0.43
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.50	0.42
1:A:313:LEU:O	1:A:325:MET:HA	2.19	0.42
1:A:467:TYR:HB3	1:A:483:HIS:O	2.19	0.42
1:A:357:PHE:HB2	5:A:800:34Q:C12	2.50	0.42
1:A:596:ARG:O	1:A:597:ARG:NH1	2.53	0.41
1:A:42:THR:HB	1:A:569:SER:OG	2.19	0.41
1:A:197:GLY:C	1:A:213:ALA:HB3	2.41	0.41
1:A:163:LYS:HG2	1:A:176:ILE:HA	2.03	0.41
1:A:167:VAL:HG11	1:A:198:ILE:HG12	2.01	0.41
1:A:550:PRO:O	1:A:551:CYS:HB3	2.21	0.41
1:A:378:GLU:CD	1:A:378:GLU:H	2.24	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.21	0.41
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.56	0.41
1:A:43:TYR:N	1:A:569:SER:OG	2.42	0.40
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.57	0.40
1:A:598:LEU:HD22	1:A:631:TYR:OH	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	727/729 (100%)	662 (91%)	59 (8%)	6 (1%)	19 51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	ARG
1	A	332	GLU
1	A	73	GLU
1	A	178	PRO
1	A	451	PRO
1	A	450	ASN

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	654/654 (100%)	565 (86%)	89 (14%)	3 11

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	56	LYS
1	A	61	ARG
1	A	63	ILE
1	A	73	GLU

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	94	THR
1	A	96	ASP
1	A	97	GLU
1	A	102	ILE
1	A	108	SER
1	A	112	GLN
1	A	114	ILE
1	A	115	LEU
1	A	122	LYS
1	A	129	THR
1	A	133	ASP
1	A	140	ARG
1	A	141	GLN
1	A	145	GLU
1	A	147	ARG
1	A	148	ILE
1	A	151	ASN
1	A	156	THR
1	A	180	LEU
1	A	182	SER
1	A	207	VAL
1	A	235	LEU
1	A	239	SER
1	A	242	SER
1	A	250	LYS
1	A	267	LYS
1	A	275	SER
1	A	276	LEU
1	A	278	SER
1	A	280	THR
1	A	286	GLN
1	A	295	ILE
1	A	308	GLN
1	A	309	GLU
1	A	312	SER
1	A	325	MET
1	A	326	ASP
1	A	334	SER
1	A	336	ARG
1	A	343	ARG
1	A	346	ILE

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Mol	Chain	Res	Type
1	A	358	ARG
1	A	360	SER
1	A	361	GLU
1	A	370	SER
1	A	385	CYS
1	A	389	ILE
1	A	395	THR
1	A	399	LYS
1	A	413	ASP
1	A	419	SER
1	A	423	LYS
1	A	435	GLN
1	A	436	LEU
1	A	437	SER
1	A	440	THR
1	A	443	THR
1	A	466	LYS
1	A	471	ARG
1	A	486	VAL
1	A	487	ASN
1	A	489	LYS
1	A	498	SER
1	A	502	LYS
1	A	521	GLU
1	A	522	THR
1	A	536	LYS
1	A	542	LEU
1	A	565	THR
1	A	589	LYS
1	A	596	ARG
1	A	614	SER
1	A	615	LYS
1	A	627	TRP
1	A	657	SER
1	A	658	ARG
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	718	GLN
1	A	736	THR
1	A	742	ILE
1	A	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	ASN
1	A	103	ASN
1	A	162	HIS
1	A	169	ASN
1	A	170	ASN
1	A	308	GLN
1	A	344	GLN
1	A	430	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	595	ASN
1	A	606	GLN
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	748	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

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	B	1	2,1	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	1.41	3 (17%)
2	MAN	B	3	2	11,11,12	0.62	0	15,15,17	1.46	1 (6%)
2	MAN	B	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.70	5 (33%)
3	NAG	C	1	3,1	14,14,15	0.76	0	17,19,21	1.84	3 (17%)
3	NAG	C	2	3	14,14,15	0.72	0	17,19,21	1.17	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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	MAN	B	3	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MAN	C2-C3	2.42	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-O5-C5	5.64	119.84	112.19
2	B	3	MAN	C1-O5-C5	4.59	118.41	112.19
2	B	2	NAG	O5-C5-C6	3.76	113.09	107.20
2	B	4	MAN	C1-O5-C5	3.60	117.08	112.19
2	B	2	NAG	C1-O5-C5	3.06	116.34	112.19
3	C	2	NAG	C4-C3-C2	2.56	114.76	111.02
3	C	1	NAG	O5-C5-C4	2.54	117.01	110.83
2	B	4	MAN	O2-C2-C3	2.51	115.16	110.14
2	B	4	MAN	O5-C5-C6	2.32	110.84	107.20
3	C	1	NAG	C3-C4-C5	2.29	114.33	110.24
2	B	4	MAN	O5-C1-C2	2.27	114.28	110.77
2	B	2	NAG	C2-N2-C7	2.11	125.91	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C3-C4-C5	2.09	113.97	110.24
2	B	4	MAN	C1-C2-C3	2.08	112.22	109.67
3	C	2	NAG	O3-C3-C4	-2.02	105.68	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1
2	B	3	MAN	C1

All (9) torsion outliers are listed below:

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

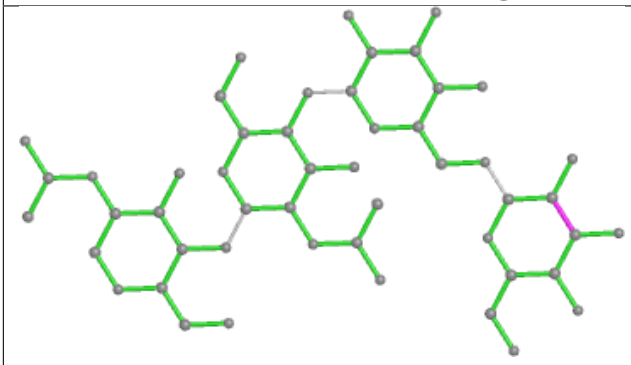
There are no ring outliers.

4 monomers are involved in 3 short contacts:

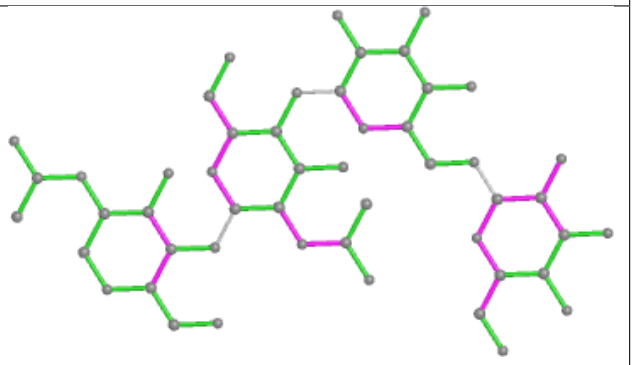
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	1	NAG	1	0
3	C	2	NAG	2	0
3	C	1	NAG	2	0

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

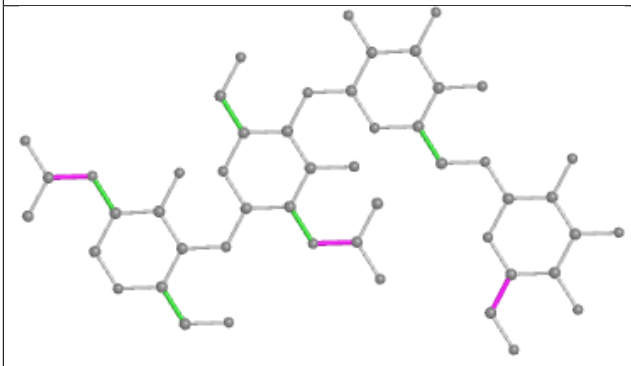
Oligosaccharide Chain B



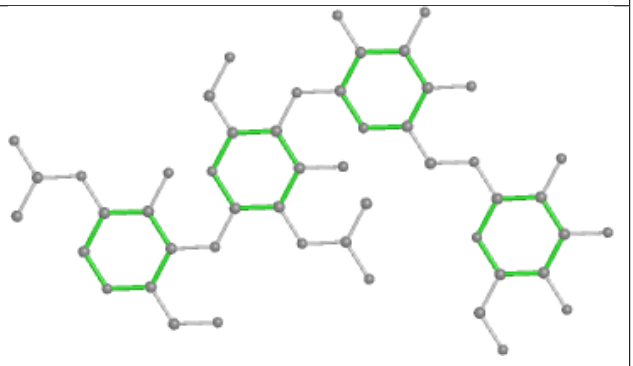
Bond lengths



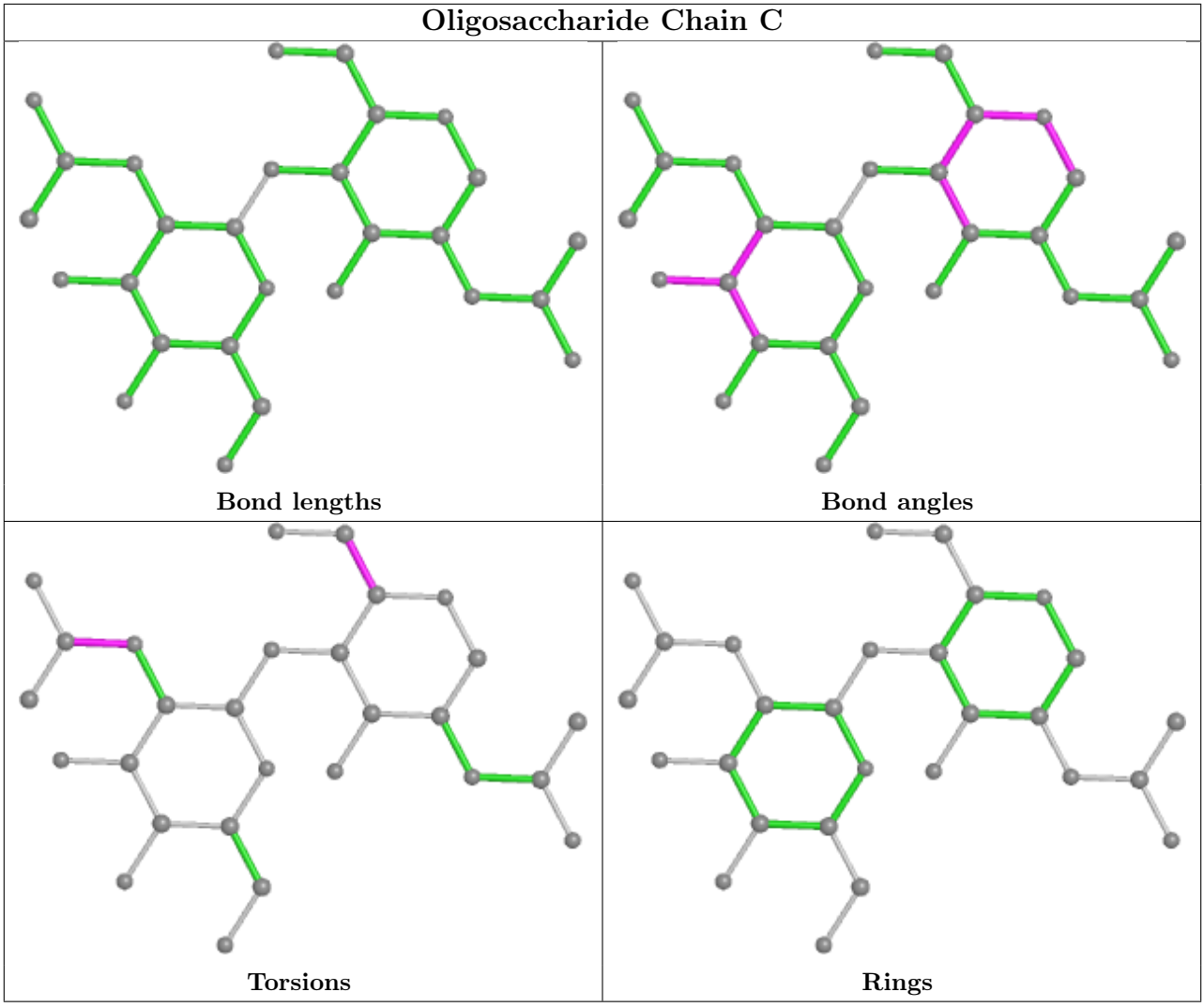
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1229	1	14,14,15	0.49	0	17,19,21	1.88	4 (23%)
5	34Q	A	800	-	28,28,28	2.46	8 (28%)	32,40,40	1.58	8 (25%)
4	NAG	A	1219	1	14,14,15	0.56	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1281	1	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
4	NAG	A	1321	1	14,14,15	0.68	0	17,19,21	1.26	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
4	NAG	A	1229	1	-	3/6/23/26	0/1/1/1
5	34Q	A	800	-	-	0/16/35/35	0/4/4/4
4	NAG	A	1219	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1281	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1321	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	34Q	C17-C10	6.62	1.62	1.50
5	A	800	34Q	C18-C17	6.34	1.52	1.39
5	A	800	34Q	C15-C14	4.02	1.48	1.41
5	A	800	34Q	C12-C13	3.82	1.48	1.41
5	A	800	34Q	C11-C16	3.70	1.47	1.38
5	A	800	34Q	C13-N5	3.26	1.43	1.37
5	A	800	34Q	C14-C13	-3.20	1.35	1.42
5	A	800	34Q	C11-C12	2.01	1.41	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1229	NAG	C1-O5-C5	5.71	119.93	112.19
5	A	800	34Q	C18-C17-C10	4.60	124.74	119.65
4	A	1321	NAG	C4-C3-C2	3.65	116.37	111.02
5	A	800	34Q	C6-C5-N2	2.79	108.43	103.44
4	A	1281	NAG	C1-O5-C5	2.59	115.69	112.19
4	A	1229	NAG	C4-C3-C2	-2.58	107.24	111.02
4	A	1229	NAG	C2-N2-C7	-2.53	119.30	122.90
5	A	800	34Q	O1-C4-C2	-2.49	117.50	121.88
5	A	800	34Q	C15-C14-C13	2.43	122.27	119.25
5	A	800	34Q	C8-C7-N2	2.27	107.51	103.44
5	A	800	34Q	C3-C2-C4	2.23	116.00	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	34Q	O2-C10-N1	-2.16	118.76	122.34
5	A	800	34Q	C17-C18-N5	-2.13	119.43	122.72
4	A	1229	NAG	O4-C4-C5	2.00	114.27	109.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1219	NAG	C8-C7-N2-C2
4	A	1219	NAG	O7-C7-N2-C2
4	A	1281	NAG	C8-C7-N2-C2
4	A	1281	NAG	O7-C7-N2-C2
4	A	1229	NAG	C8-C7-N2-C2
4	A	1219	NAG	O5-C5-C6-O6
4	A	1229	NAG	O7-C7-N2-C2
4	A	1321	NAG	O5-C5-C6-O6
4	A	1219	NAG	C4-C5-C6-O6
4	A	1281	NAG	O5-C5-C6-O6
4	A	1281	NAG	C4-C5-C6-O6
4	A	1321	NAG	C4-C5-C6-O6
4	A	1229	NAG	C4-C5-C6-O6

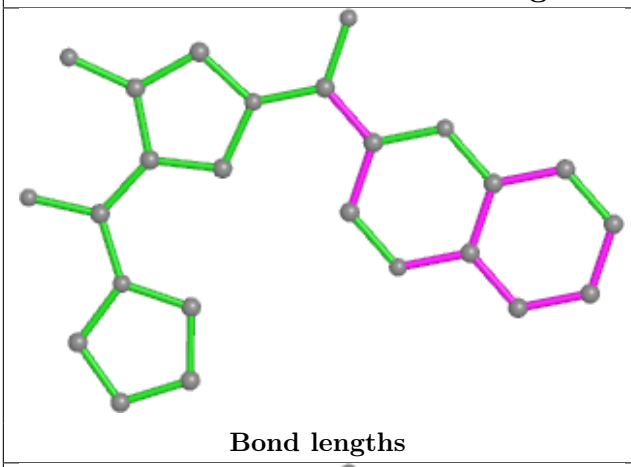
There are no ring outliers.

2 monomers are involved in 2 short contacts:

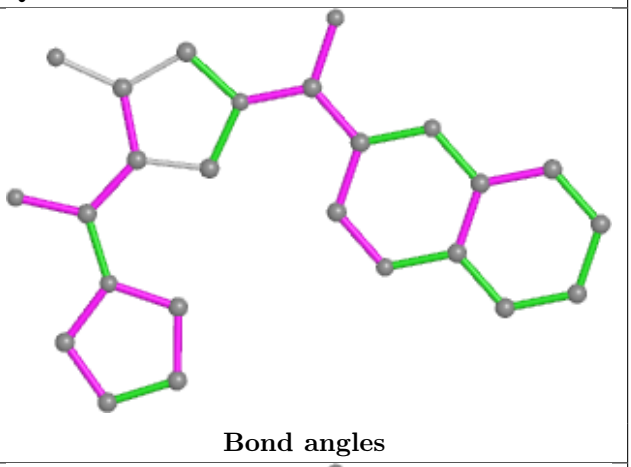
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	34Q	1	0
4	A	1219	NAG	1	0

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

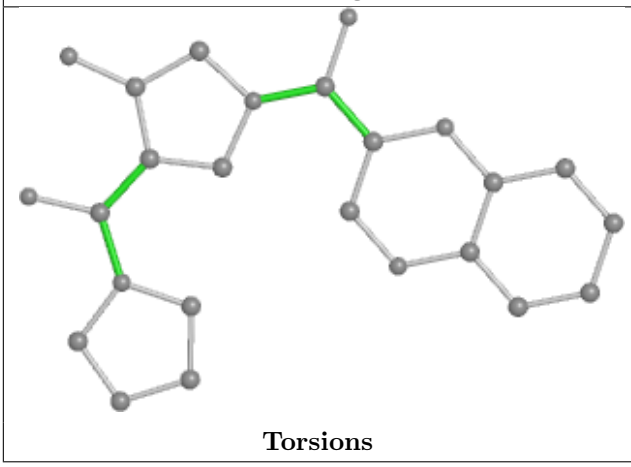
Ligand 34Q A 800



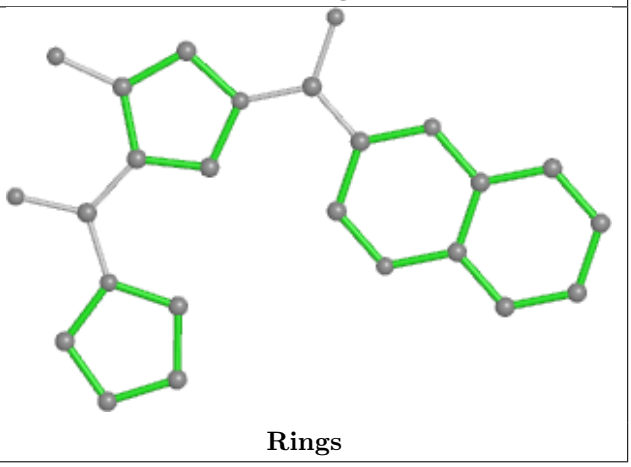
Bond lengths



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

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	729/729 (100%)	-0.22	3 (0%) 92 93	13, 37, 59, 80	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	2.2
1	A	73	GLU	2.2
1	A	99	GLY	2.1

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

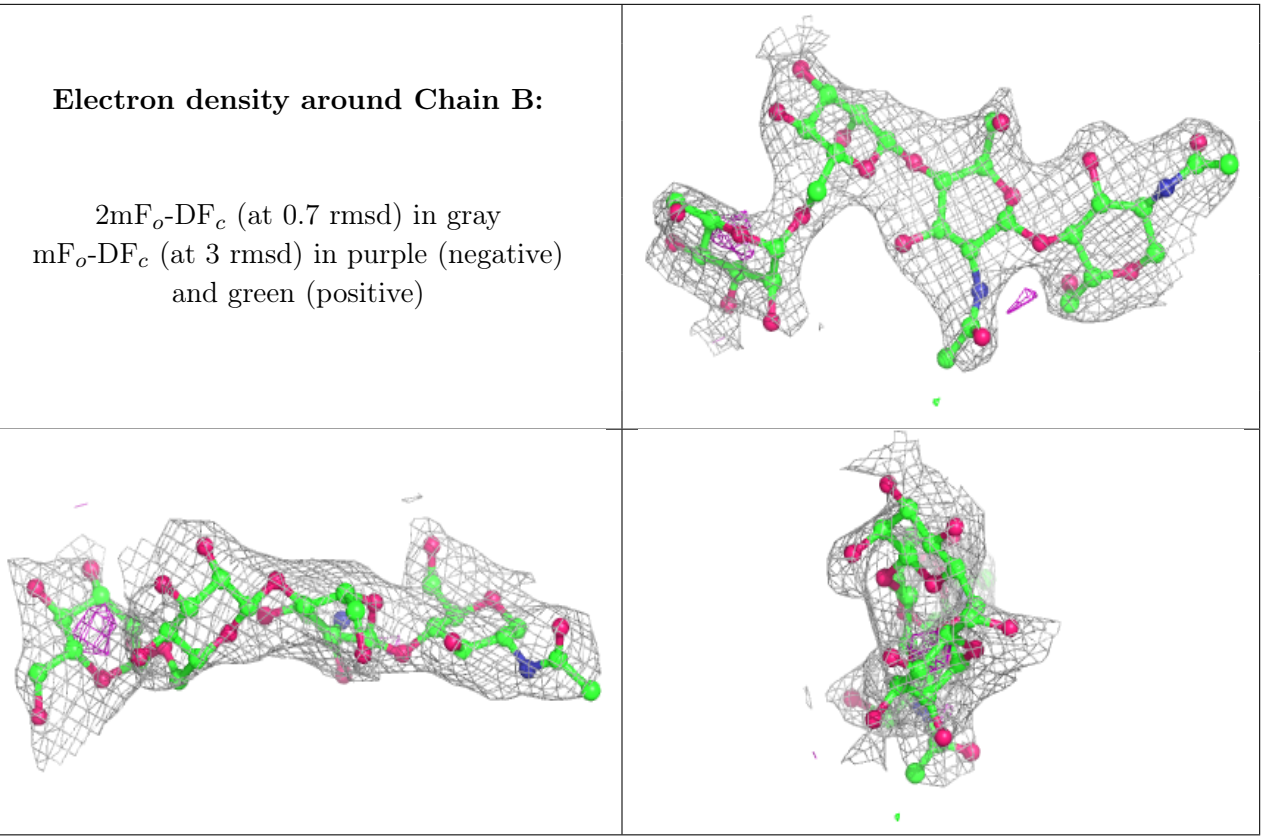
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B	4	11/12	0.71	0.43	87,89,89,89	0
2	MAN	B	3	11/12	0.77	0.28	77,79,83,86	0
3	NAG	C	2	14/15	0.85	0.28	74,77,78,80	0
3	NAG	C	1	14/15	0.87	0.28	61,65,67,71	0
2	NAG	B	2	14/15	0.93	0.23	64,68,70,73	0
2	NAG	B	1	14/15	0.94	0.20	45,49,53,59	0

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

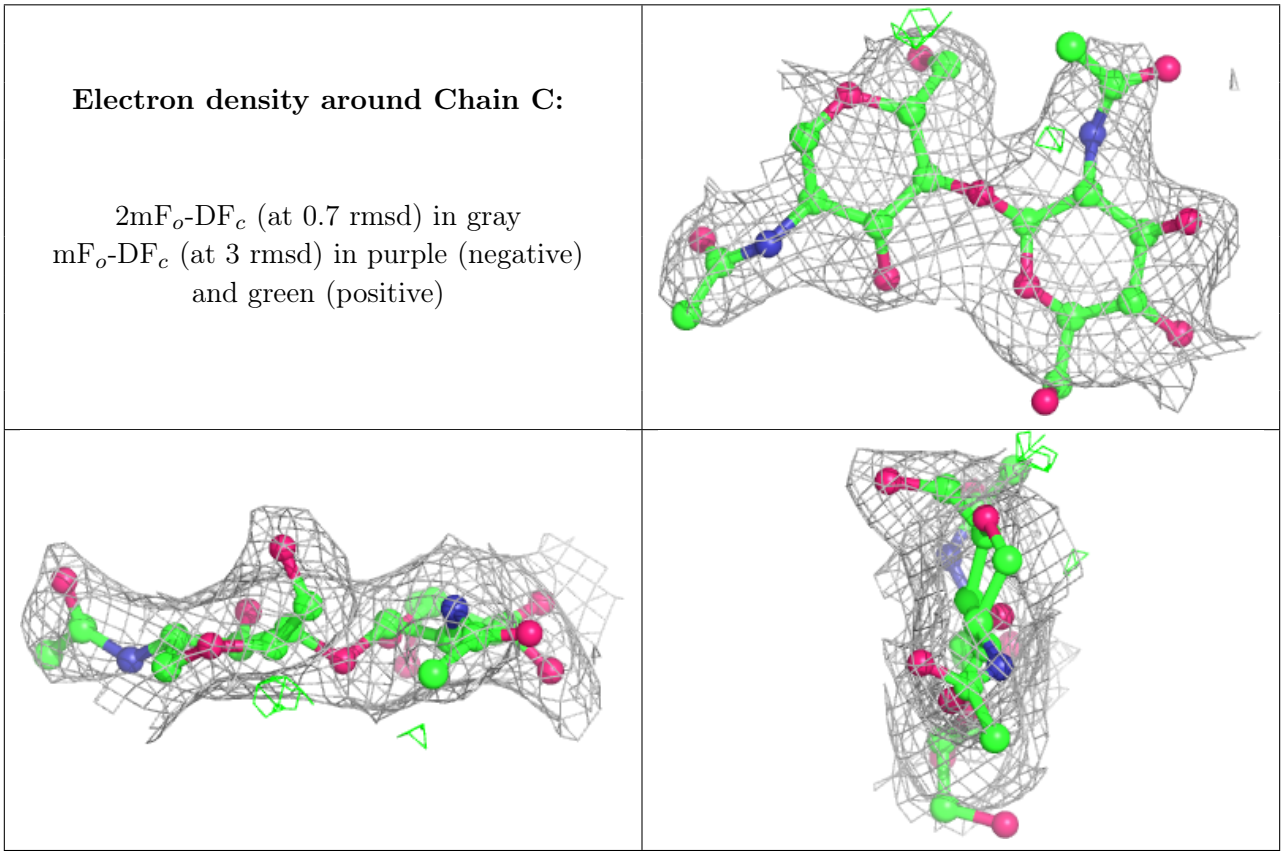
Electron density around Chain B:

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



Electron density around Chain C:

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



6.4 Ligands

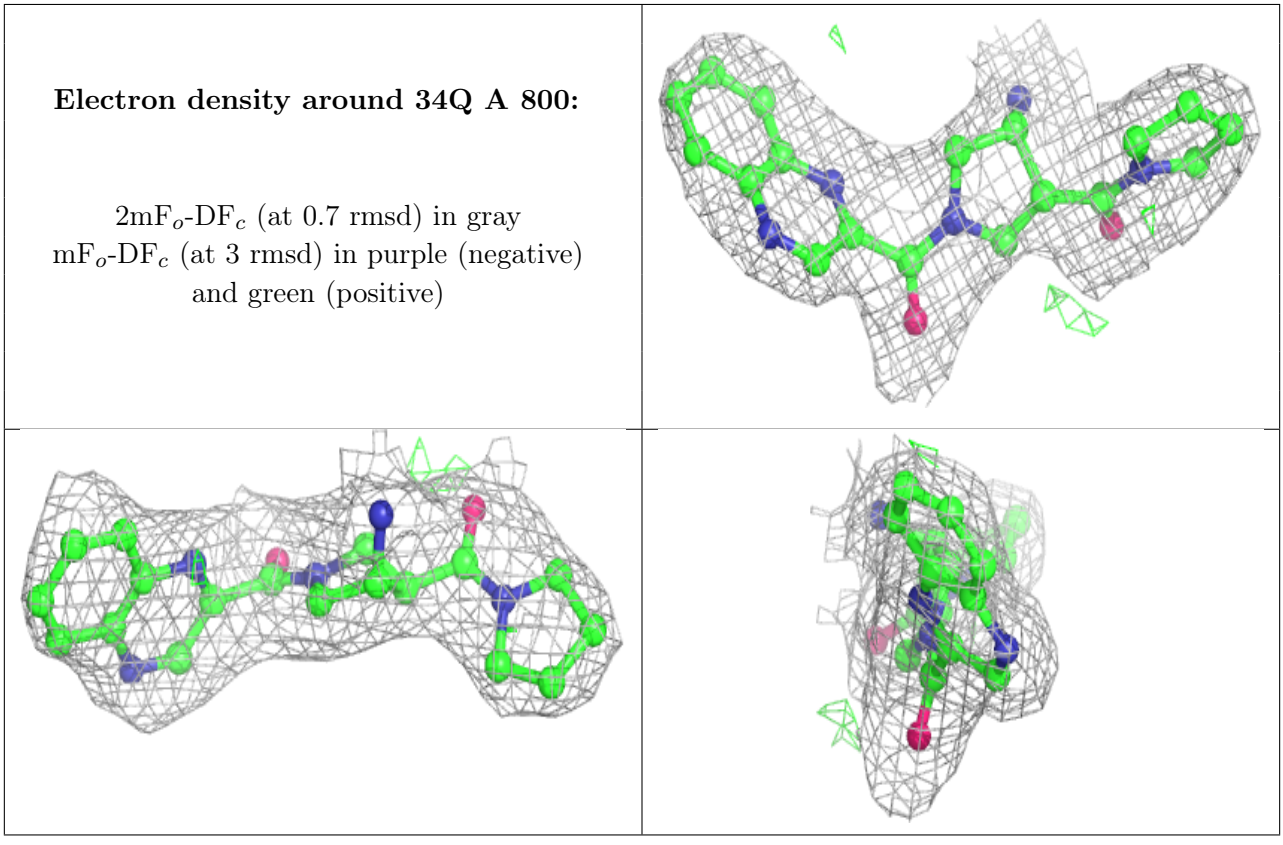
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	A	1321	14/15	0.83	0.26	58,63,64,66	0
4	NAG	A	1219	14/15	0.84	0.24	64,66,67,67	0
4	NAG	A	1281	14/15	0.89	0.24	62,64,66,66	0
4	NAG	A	1229	14/15	0.90	0.18	39,48,52,54	0
5	34Q	A	800	25/25	0.95	0.24	27,33,39,39	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 34Q A 800:

$2mF_o$-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

There are no such residues in this entry.