



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:20 PM BST

PDB ID : 3KM4
Title : Optimization of Orally Bioavailable Alkyl Amine Renin Inhibitors
Authors : Wu, Z.; McKeever, B.M.
Deposited on : 2009-11-09
Resolution : 1.90 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 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

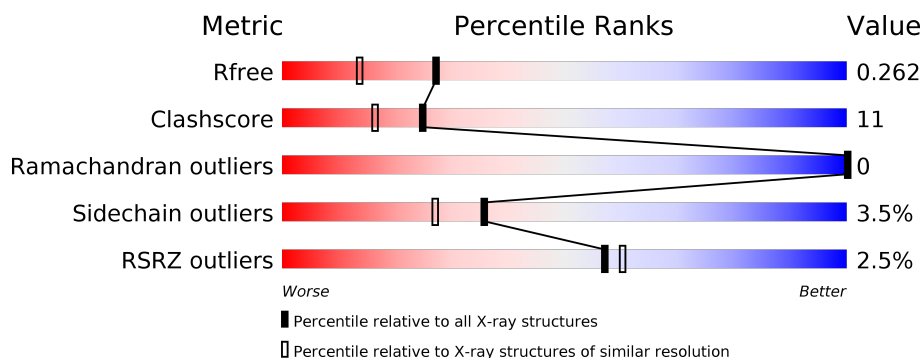
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 $\leq 5\%$. 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	337	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	337	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5815 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 Renin.

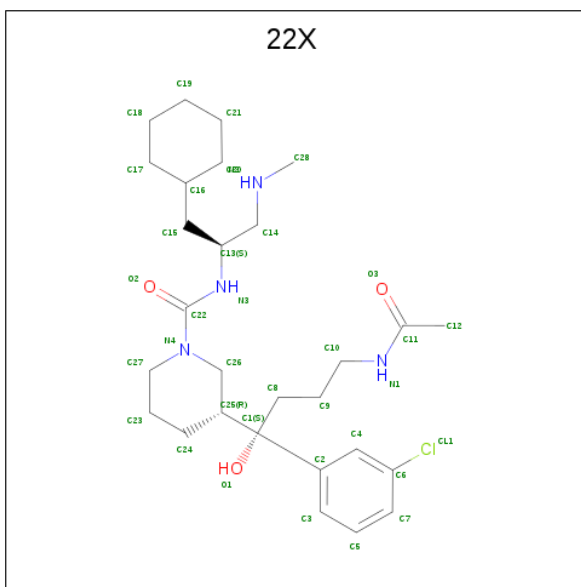
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2598	1656	421	507	14			
1	B	333	Total	C	N	O	S	0	0	0
			2569	1641	416	498	14			

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



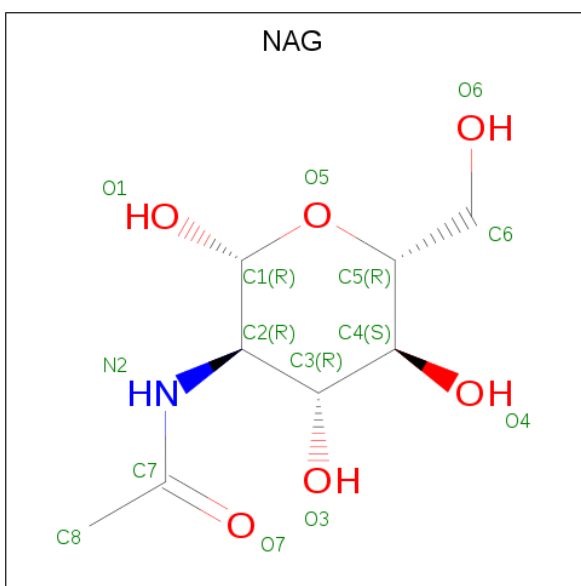
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is (3R)-3-[(1S)-4-(acetlamino)-1-(3-chlorophenyl)-1-hydroxybutyl]-N-{(1S)-2-cyclohexyl-1-[(methylamino)methyl]ethyl}piperidine-1-carboxamide (three-letter code: 22X) (formula: C₂₈H₄₅ClN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			36	28	1	4	3		
3	A	1	Total	C	Cl	N	O	0	0
			36	28	1	4	3		
3	B	1	Total	C	Cl	N	O	0	0
			36	28	1	4	3		
3	B	1	Total	C	Cl	N	O	0	0
			36	28	1	4	3		

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

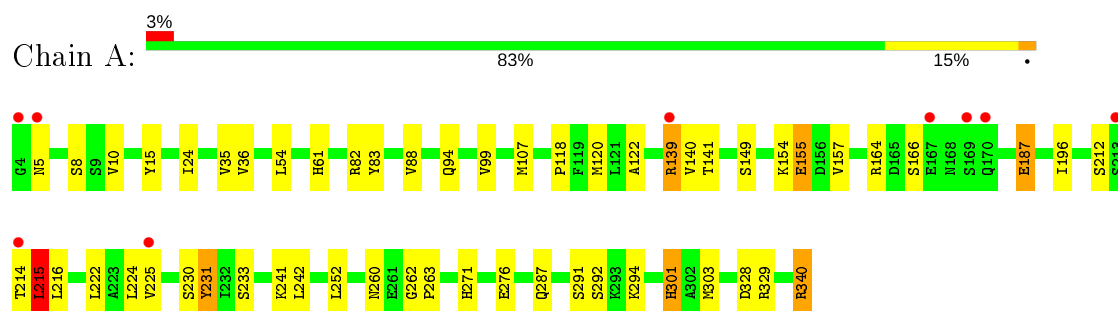
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total	O	0	0
			227	227		
5	B	235	Total	O	0	0
			235	235		

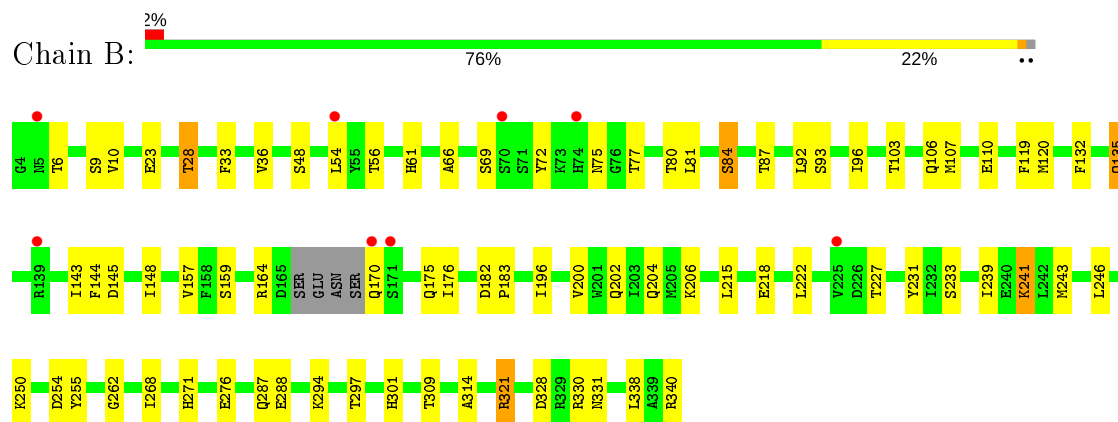
3 Residue-property plots [i](#)

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.

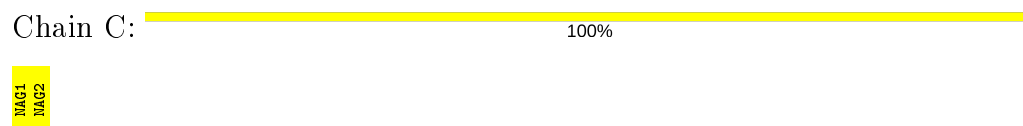
- Molecule 1: Renin



- Molecule 1: Renin



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.83Å 96.94Å 148.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 29.13 – 1.70	Depositor EDS
% Data completeness (in resolution range)	82.2 (50.00-1.90) 83.4 (29.13-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.261 0.202 , 0.262	Depositor DCC
R_{free} test set	3607 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, 22X

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	4/2658 (0.2%)	1.01	3/3604 (0.1%)
1	B	1.08	0/2628	0.96	2/3562 (0.1%)
All	All	1.08	4/5286 (0.1%)	0.99	5/7166 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TYR	CD1-CE1	-7.19	1.28	1.39
1	A	35	VAL	CB-CG1	5.97	1.65	1.52
1	A	88	VAL	CB-CG2	-5.11	1.42	1.52
1	A	231	TYR	CD2-CE2	-5.06	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LEU	CA-CB-CG	9.00	136.00	115.30
1	B	338	LEU	CA-CB-CG	7.83	133.31	115.30
1	B	321	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	329	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	224	LEU	CB-CG-CD2	-5.21	102.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	VAL	Peptide
1	B	6	THR	Peptide

5.2 Too-close contacts

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	2598	0	2523	52	0
1	B	2569	0	2500	62	0
2	C	28	0	25	0	0
3	A	72	0	89	15	0
3	B	72	0	90	6	0
4	B	14	0	13	0	0
5	A	227	0	0	6	0
5	B	235	0	0	5	0
All	All	5815	0	5240	114	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 11.

All (114) 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:B:9:SER:HB2	1:B:175:GLN:NE2	1.61	1.16
1:A:231:TYR:H	3:A:341:22X:H12A	1.19	1.08
1:B:9:SER:HB2	1:B:175:GLN:HE21	0.89	1.06
1:B:231:TYR:H	3:B:341:22X:H12A	1.25	0.97
1:B:330:ARG:HH11	1:B:331:ASN:HD21	1.13	0.96
1:B:9:SER:CB	1:B:175:GLN:HE21	1.79	0.95
1:A:5:ASN:OD1	1:A:154:LYS:HD3	1.69	0.92
1:B:170:GLN:OE1	5:B:466:HOH:O	1.89	0.90
1:B:9:SER:CB	1:B:175:GLN:NE2	2.35	0.90
1:A:231:TYR:N	3:A:341:22X:H12A	1.94	0.82
1:A:262:GLY:HA3	1:A:287:GLN:HE22	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:HIS:HD2	1:A:276:GLU:OE2	1.65	0.80
1:A:82:ARG:NH2	1:B:294:LYS:HE2	2.06	0.70
1:A:82:ARG:HH22	1:B:294:LYS:HE2	1.57	0.69
1:A:83:TYR:HB3	5:A:496:HOH:O	1.92	0.69
1:B:204:GLN:HG2	1:B:206:LYS:NZ	2.07	0.69
1:B:196:ILE:CD1	1:B:222:LEU:HD22	2.23	0.68
3:B:400:22X:H26A	3:B:341:22X:H12B	1.75	0.68
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.59	0.67
1:A:252:LEU:HD22	1:B:84:SER:HB3	1.76	0.67
1:A:231:TYR:H	3:A:341:22X:C12	2.04	0.66
1:B:231:TYR:N	3:B:341:22X:H12A	2.06	0.65
1:A:271:HIS:CD2	1:A:276:GLU:OE2	2.51	0.63
1:A:230:SER:H	3:A:341:22X:C12	2.11	0.63
1:B:132:PHE:H	1:B:135:GLN:NE2	1.96	0.63
1:B:330:ARG:NH1	1:B:331:ASN:HD21	1.94	0.63
1:A:215:LEU:HD23	1:A:216:LEU:HG	1.80	0.62
1:A:303:MET:CE	5:A:424:HOH:O	2.48	0.62
1:B:231:TYR:H	3:B:341:22X:C12	2.04	0.62
1:A:118:PRO:HG2	3:A:400:22X:CL1	2.39	0.60
1:A:230:SER:N	3:A:341:22X:C12	2.66	0.59
1:A:155:GLU:HB3	1:A:157:VAL:HG13	1.86	0.58
1:B:330:ARG:HH11	1:B:331:ASN:ND2	1.93	0.58
1:A:301:HIS:CE1	3:A:341:22X:N1	2.72	0.58
3:A:400:22X:H26A	3:A:341:22X:H12B	1.86	0.58
1:B:92:LEU:HD13	1:B:107:MET:CE	2.33	0.57
1:A:301:HIS:HE1	3:A:341:22X:N1	2.02	0.57
1:A:242:LEU:C	1:A:242:LEU:HD23	2.25	0.57
1:A:301:HIS:CE1	3:A:341:22X:H10A	2.40	0.57
1:A:216:LEU:CD2	1:A:241:LYS:HB2	2.35	0.56
1:B:66:ALA:HB1	1:B:72:TYR:CD1	2.40	0.56
1:B:164:ARG:HD2	1:B:321:ARG:HD2	1.86	0.56
1:A:262:GLY:HA3	1:A:287:GLN:NE2	2.17	0.55
1:A:187:GLU:HB2	1:A:340:ARG:NH1	2.21	0.54
1:A:61:HIS:HE1	1:A:122:ALA:O	1.90	0.54
1:B:262:GLY:HA3	1:B:287:GLN:OE1	2.10	0.51
1:A:216:LEU:HD21	1:A:241:LYS:HB2	1.91	0.51
1:B:250:LYS:CE	5:B:486:HOH:O	2.58	0.51
1:B:271:HIS:HD2	1:B:276:GLU:OE2	1.93	0.50
1:B:96:ILE:CG2	1:B:103:THR:CG2	2.89	0.50
1:B:36:VAL:HG21	3:B:400:22X:H10A	1.93	0.50
1:A:216:LEU:HD11	1:A:242:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:341:22X:C22	3:A:341:22X:H16	2.40	0.50
1:B:200:VAL:HG22	1:B:202:GLN:HB2	1.93	0.49
1:A:36:VAL:HG21	3:A:400:22X:H10A	1.94	0.49
1:B:80:THR:HG23	1:B:87:THR:HG23	1.95	0.49
1:A:5:ASN:HA	1:A:154:LYS:HG2	1.96	0.48
1:A:291:SER:HB3	1:A:294:LYS:HG2	1.94	0.48
1:B:143:ILE:HG23	1:B:144:PHE:N	2.29	0.48
1:B:233:SER:HA	1:B:301:HIS:O	2.13	0.48
1:B:164:ARG:CD	1:B:321:ARG:HD2	2.43	0.48
1:B:48:SER:HB2	1:B:110:GLU:HB3	1.96	0.48
1:A:328:ASP:C	1:A:328:ASP:OD1	2.52	0.48
1:B:159:SER:O	1:B:176:ILE:HA	2.14	0.48
1:B:204:GLN:HG2	1:B:206:LYS:HZ1	1.78	0.47
1:B:254:ASP:HB2	1:B:297:THR:HG23	1.96	0.47
1:A:149:SER:HB2	5:A:452:HOH:O	2.14	0.47
1:A:94:GLN:NE2	5:A:545:HOH:O	2.37	0.47
1:B:92:LEU:HD13	1:B:107:MET:HE2	1.96	0.47
1:B:56:THR:HG22	1:B:120:MET:CE	2.44	0.47
1:A:107:MET:HB3	1:A:140:VAL:HG13	1.97	0.47
1:B:309:THR:HB	5:B:567:HOH:O	2.14	0.47
1:B:157:VAL:HG12	1:B:328:ASP:HA	1.96	0.46
1:B:250:LYS:HE3	5:B:486:HOH:O	2.15	0.46
1:B:196:ILE:HD11	1:B:222:LEU:HD22	1.96	0.46
1:B:92:LEU:HD13	1:B:107:MET:HE3	1.96	0.46
1:A:303:MET:HE2	5:A:424:HOH:O	2.14	0.45
1:A:301:HIS:CE1	3:A:341:22X:C10	2.99	0.45
1:A:139:ARG:HG3	1:A:139:ARG:NH1	2.27	0.45
1:B:243:MET:HG3	1:B:255:TYR:CE1	2.52	0.45
1:A:24:ILE:HG22	1:A:99:VAL:HG13	1.99	0.45
1:B:196:ILE:HD13	1:B:222:LEU:HD22	1.96	0.44
1:B:246:LEU:HD11	1:B:268:ILE:HD11	1.98	0.44
1:B:28:THR:O	1:B:69:SER:HA	2.16	0.44
1:B:106:GLN:OE1	1:B:143:ILE:HA	2.18	0.44
1:B:233:SER:OG	1:B:314:ALA:HB3	2.18	0.44
1:B:81:LEU:O	1:B:87:THR:HA	2.18	0.44
1:A:196:ILE:HD11	1:A:222:LEU:HD22	1.99	0.43
1:B:56:THR:CG2	1:B:120:MET:HE2	2.47	0.43
1:A:54:LEU:N	1:A:54:LEU:HD12	2.33	0.43
1:B:227:THR:O	3:B:400:22X:H12A	2.19	0.43
1:B:145:ASP:HA	1:B:148:ILE:HD12	2.01	0.43
1:A:187:GLU:HB2	1:A:340:ARG:HH12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MET:HE1	5:A:424:HOH:O	2.13	0.43
1:B:93:SER:O	1:B:107:MET:HG3	2.19	0.43
1:A:10:VAL:HG21	1:A:99:VAL:HG12	2.01	0.43
1:B:10:VAL:HB	1:B:176:ILE:CG2	2.49	0.42
1:B:56:THR:HG21	1:B:120:MET:HE2	2.02	0.42
1:A:61:HIS:CE1	1:A:122:ALA:O	2.72	0.42
1:A:120:MET:HB3	1:A:120:MET:HE3	1.86	0.42
1:A:230:SER:H	3:A:341:22X:H12B	1.82	0.41
1:B:182:ASP:HA	1:B:183:PRO:HD2	1.86	0.41
1:B:75:ASN:OD1	1:B:77:THR:OG1	2.33	0.41
1:B:23:GLU:HA	1:B:33:PHE:O	2.20	0.41
1:A:233:SER:HA	1:A:301:HIS:O	2.20	0.41
1:B:61:HIS:HE1	1:B:119:PHE:O	2.04	0.41
1:B:215:LEU:HD11	1:B:241:LYS:HG2	2.03	0.41
1:A:260:ASN:OD1	1:A:292:SER:HA	2.20	0.41
1:A:230:SER:N	3:A:341:22X:H12	2.36	0.40
1:A:107:MET:HB3	1:A:140:VAL:CG1	2.51	0.40
1:A:54:LEU:HD12	1:A:54:LEU:H	1.85	0.40
1:B:340:ARG:NH1	5:B:395:HOH:O	2.53	0.40
1:B:204:GLN:HG2	1:B:206:LYS:HZ2	1.81	0.40
1:B:239:ILE:HD13	1:B:239:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	335/337 (99%)	326 (97%)	9 (3%)	0	100	100
1	B	329/337 (98%)	321 (98%)	8 (2%)	0	100	100
All	All	664/674 (98%)	647 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	287/287 (100%)	274 (96%)	13 (4%)	27	18
1	B	283/287 (99%)	276 (98%)	7 (2%)	47	41
All	All	570/574 (99%)	550 (96%)	20 (4%)	36	27

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	139	ARG
1	A	141	THR
1	A	155	GLU
1	A	164	ARG
1	A	166	SER
1	A	187	GLU
1	A	212	SER
1	A	214	THR
1	A	215	LEU
1	A	263	PRO
1	A	301	HIS
1	A	340	ARG
1	B	28	THR
1	B	54	LEU
1	B	84	SER
1	B	135	GLN
1	B	218	GLU
1	B	241	LYS
1	B	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	271	HIS
1	A	287	GLN
1	A	301	HIS
1	A	331	ASN
1	A	332	ASN
1	B	135	GLN
1	B	146	ASN
1	B	175	GLN
1	B	204	GLN
1	B	271	HIS
1	B	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	1,2	14,14,15	0.92	0	17,19,21	1.63	5 (29%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	2.50	5 (29%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	2	NAG	C1-O5-C5	7.32	122.11	112.19
2	C	2	NAG	C3-C4-C5	3.85	117.10	110.24
2	C	1	NAG	C2-N2-C7	3.32	127.63	122.90
2	C	2	NAG	C6-C5-C4	-3.25	105.39	113.00
2	C	2	NAG	O5-C5-C4	2.99	118.10	110.83
2	C	1	NAG	O5-C1-C2	2.79	115.70	111.29
2	C	2	NAG	O5-C5-C6	2.61	111.30	107.20
2	C	1	NAG	O4-C4-C3	-2.33	104.97	110.35
2	C	1	NAG	C4-C3-C2	-2.14	107.88	111.02
2	C	1	NAG	C8-C7-N2	-2.13	112.49	116.10

There are no chirality outliers.

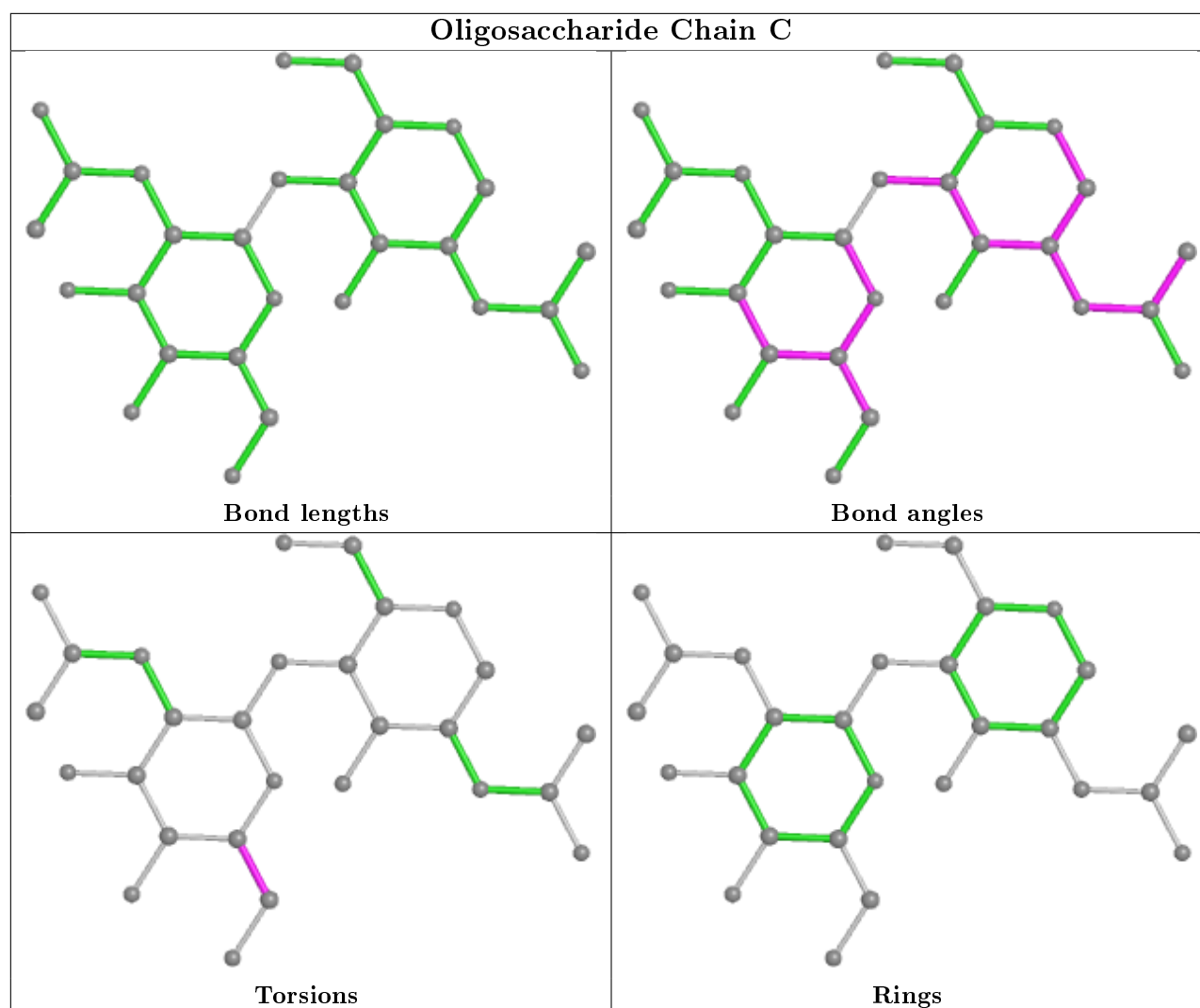
All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry ⓘ

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
3	22X	A	400	-	36,38,38	1.00	3 (8%)	38,51,51	2.07	13 (34%)
3	22X	B	341	-	36,38,38	1.03	2 (5%)	38,51,51	2.17	12 (31%)
3	22X	A	341	-	36,38,38	1.22	5 (13%)	38,51,51	2.37	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	600	1	14,14,15	0.74	1 (7%)	17,19,21	1.16	1 (5%)
3	22X	B	400	-	36,38,38	1.29	4 (11%)	38,51,51	1.93	6 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	22X	A	400	-	-	8/35/53/53	0/3/3/3
3	22X	B	341	-	-	6/35/53/53	0/3/3/3
3	22X	A	341	-	-	5/35/53/53	0/3/3/3
4	NAG	B	600	1	-	2/6/23/26	0/1/1/1
3	22X	B	400	-	-	3/35/53/53	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	341	22X	C15-C16	3.30	1.58	1.53
3	B	400	22X	C27-N4	-3.00	1.41	1.47
3	A	341	22X	C1-C2	-2.65	1.49	1.52
3	A	341	22X	O1-C1	-2.61	1.39	1.43
3	B	341	22X	C12-C11	-2.53	1.45	1.50
3	B	400	22X	C6-CL1	2.41	1.79	1.74
3	A	400	22X	C4-C6	2.41	1.42	1.38
3	B	400	22X	C3-C2	2.35	1.43	1.39
4	B	600	NAG	C1-C2	2.33	1.55	1.52
3	B	341	22X	C10-N1	2.23	1.51	1.46
3	A	341	22X	O3-C11	2.16	1.28	1.23
3	A	400	22X	C22-N4	-2.07	1.32	1.36
3	A	341	22X	C26-C25	2.05	1.55	1.53
3	B	400	22X	C23-C27	2.03	1.58	1.51
3	A	400	22X	C23-C24	2.00	1.58	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	341	22X	C10-N1-C11	8.13	135.05	122.56
3	A	341	22X	C6-C4-C2	-7.08	115.02	119.62
3	B	341	22X	C6-C4-C2	-6.48	115.41	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	22X	C23-C27-N4	-6.46	97.91	110.66
3	A	400	22X	C23-C27-N4	-6.01	98.79	110.66
3	B	341	22X	C5-C3-C2	4.92	125.93	120.76
3	A	341	22X	C8-C9-C10	-4.71	104.28	112.46
3	B	400	22X	C9-C10-N1	-4.65	98.92	112.21
3	A	400	22X	C6-C4-C2	-4.15	116.92	119.62
3	B	400	22X	C5-C3-C2	3.91	124.86	120.76
3	A	400	22X	C5-C3-C2	3.88	124.83	120.76
3	B	341	22X	C4-C6-CL1	-3.86	114.33	119.15
3	A	400	22X	C10-N1-C11	3.79	128.39	122.56
3	B	400	22X	C7-C6-C4	3.36	125.99	121.53
3	A	341	22X	C4-C6-CL1	-3.29	115.04	119.15
3	B	341	22X	C10-N1-C11	3.26	127.57	122.56
3	B	341	22X	C7-C6-C4	3.25	125.85	121.53
3	A	400	22X	C7-C6-C4	3.11	125.66	121.53
3	B	341	22X	C7-C5-C3	-3.04	115.93	120.25
3	B	341	22X	C8-C9-C10	-3.00	107.25	112.46
3	A	400	22X	C19-C21-C20	-2.98	105.34	111.42
3	B	400	22X	C18-C17-C16	-2.89	106.69	112.15
3	B	341	22X	O3-C11-C12	-2.82	116.81	122.06
3	B	341	22X	C13-N3-C22	2.74	126.82	122.20
3	A	341	22X	C13-N3-C22	2.72	126.79	122.20
3	A	400	22X	C24-C25-C26	-2.62	103.63	108.67
3	A	400	22X	C18-C17-C16	-2.61	107.22	112.15
3	B	341	22X	C23-C24-C25	-2.54	107.81	112.23
3	A	341	22X	O1-C1-C2	-2.50	104.13	109.06
3	A	341	22X	N3-C22-N4	2.41	121.60	117.21
3	A	400	22X	C15-C13-C14	2.38	117.30	109.66
3	B	400	22X	C12-C11-N1	2.37	120.28	116.09
3	A	400	22X	C24-C23-C27	-2.34	107.57	110.85
3	A	341	22X	C3-C2-C4	2.32	122.23	117.76
3	A	341	22X	C7-C6-C4	2.21	124.46	121.53
3	A	400	22X	C27-N4-C26	-2.15	108.74	113.06
3	B	341	22X	O3-C11-N1	2.12	127.72	121.74
4	B	600	NAG	O5-C5-C6	2.12	110.52	107.20
3	B	341	22X	C19-C21-C20	2.08	115.65	111.42
3	A	400	22X	C21-C19-C18	-2.05	104.87	111.18
3	A	400	22X	O1-C1-C2	-2.03	105.07	109.06

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	22X	O1-C1-C8-C9
3	A	400	22X	C2-C1-C8-C9
3	B	341	22X	C15-C13-N3-C22
3	A	341	22X	C15-C13-N3-C22
4	B	600	NAG	O5-C5-C6-O6
3	B	341	22X	O3-C11-N1-C10
3	B	341	22X	C12-C11-N1-C10
3	A	341	22X	O3-C11-N1-C10
3	A	341	22X	C12-C11-N1-C10
3	A	400	22X	N3-C13-C14-N2
3	B	400	22X	N3-C13-C14-N2
3	A	400	22X	C15-C13-C14-N2
3	B	400	22X	C15-C13-C14-N2
3	B	341	22X	C13-C15-C16-C17
3	B	341	22X	C13-C15-C16-C20
3	A	341	22X	N3-C13-C15-C16
3	A	400	22X	C25-C1-C8-C9
4	B	600	NAG	C4-C5-C6-O6
3	A	400	22X	C13-C14-N2-C28
3	B	400	22X	N1-C10-C9-C8
3	A	341	22X	C14-C13-N3-C22
3	B	341	22X	C14-C13-N3-C22
3	A	400	22X	C8-C1-C2-C3
3	A	400	22X	C8-C1-C2-C4

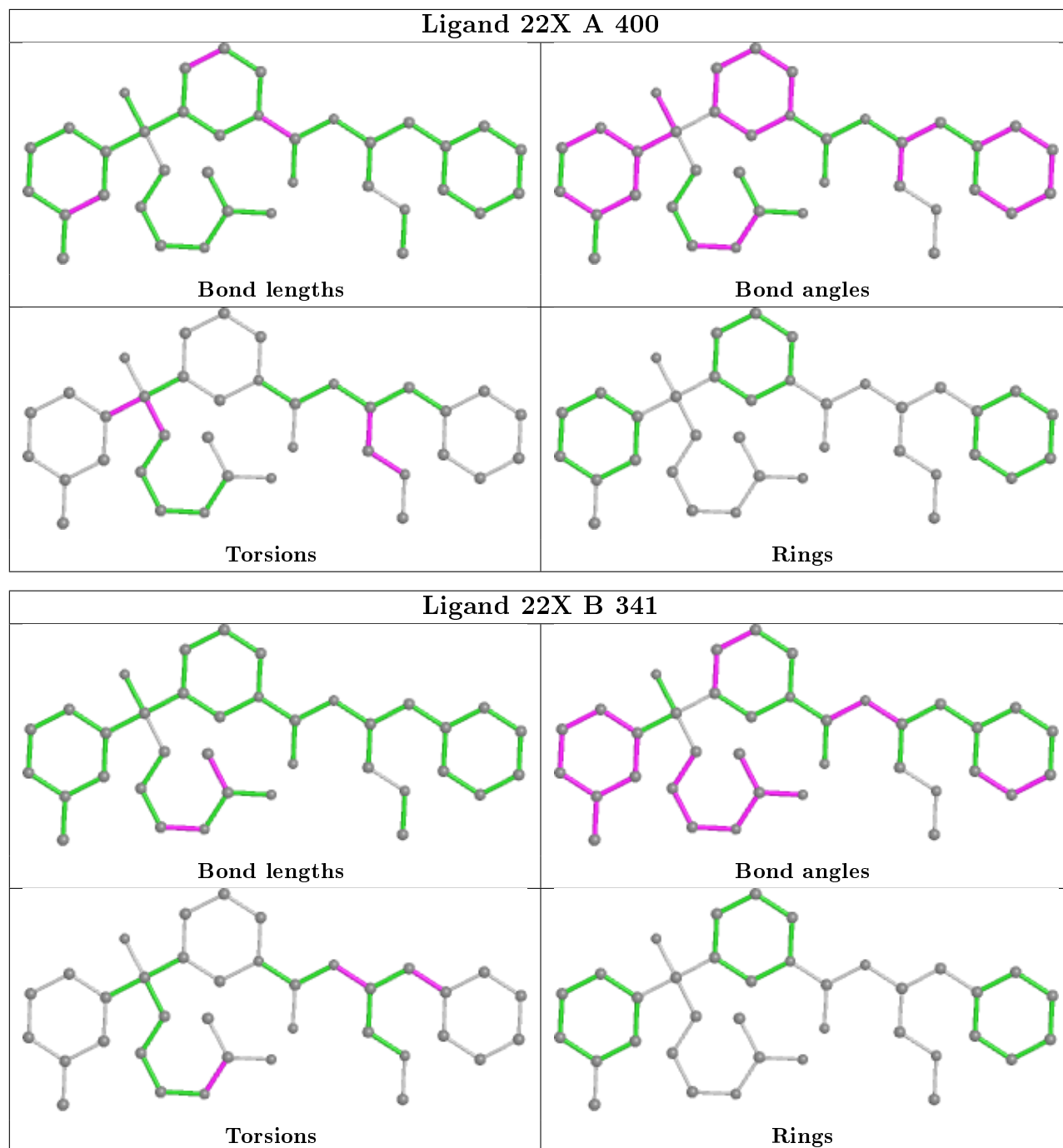
There are no ring outliers.

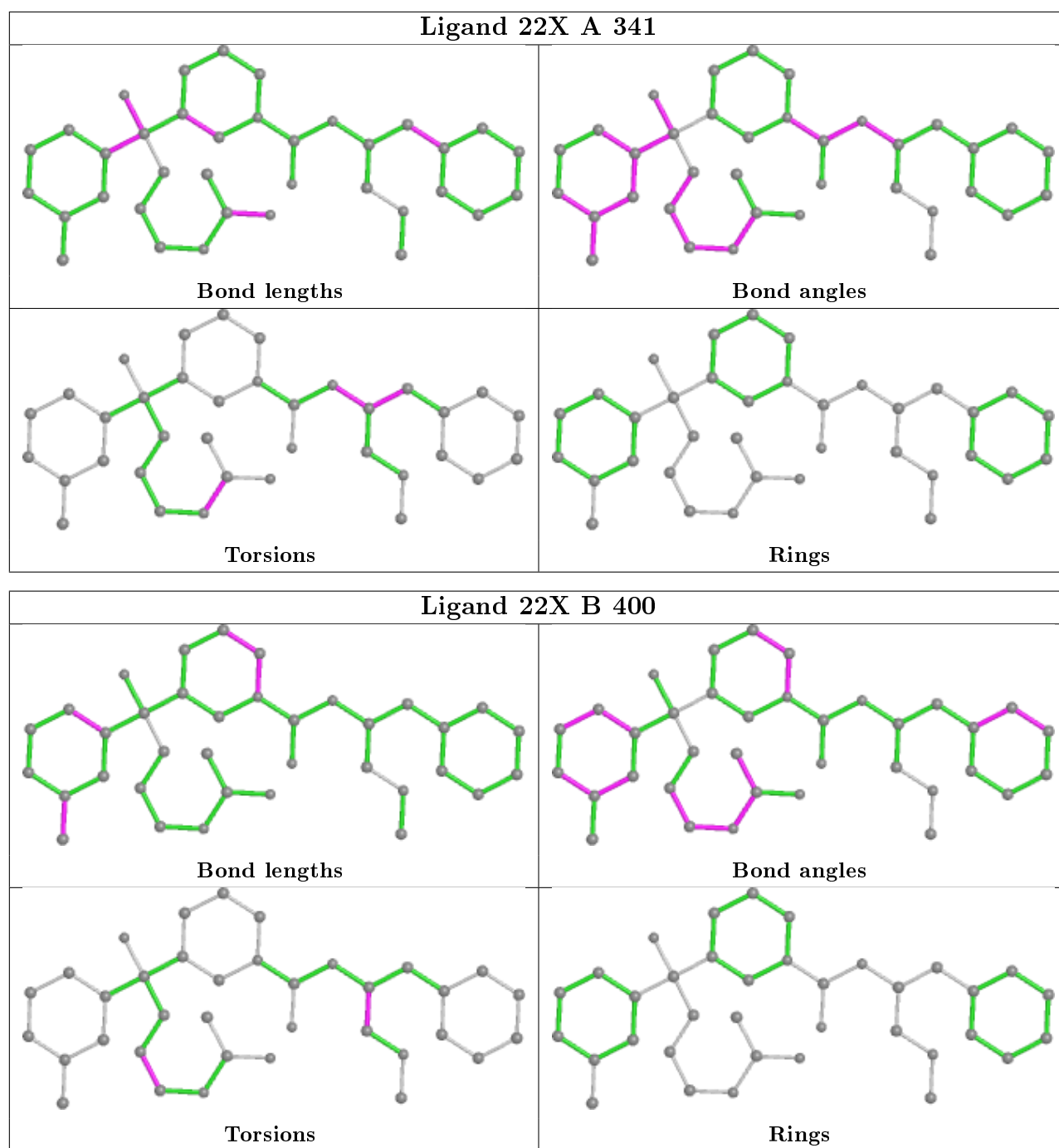
4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	22X	3	0
3	B	341	22X	4	0
3	A	341	22X	13	0
3	B	400	22X	3	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 than 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.





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, 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(Å ²)	Q<0.9
1	A	337/337 (100%)	-0.17	9 (2%) 54 57	15, 26, 41, 53	0
1	B	333/337 (98%)	-0.12	8 (2%) 59 62	14, 25, 46, 54	0
All	All	670/674 (99%)	-0.15	17 (2%) 57 60	14, 26, 43, 54	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	LEU	4.0
1	A	170	GLN	3.8
1	A	169	SER	3.5
1	B	171	SER	3.2
1	A	5	ASN	3.1
1	A	4	GLY	2.8
1	B	5	ASN	2.6
1	A	139	ARG	2.5
1	B	170	GLN	2.5
1	B	139	ARG	2.5
1	B	225	VAL	2.5
1	A	213	SER	2.4
1	A	167	GLU	2.1
1	A	214	THR	2.1
1	B	70	SER	2.1
1	A	225	VAL	2.0
1	B	74	HIS	2.0

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

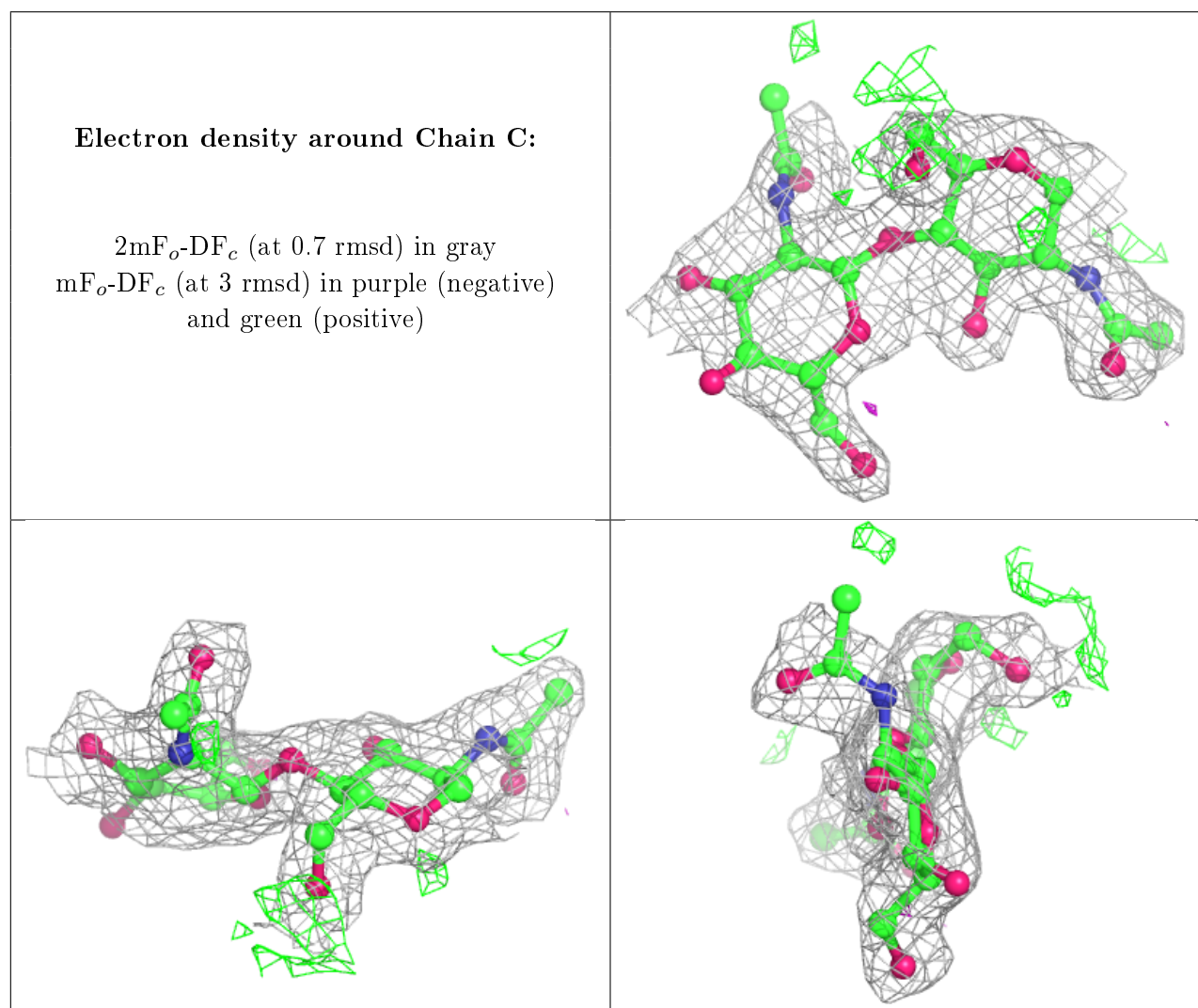
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.84	0.22	46,52,57,58	0
2	NAG	C	1	14/15	0.93	0.09	28,36,43,44	0

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



6.4 Ligands [i](#)

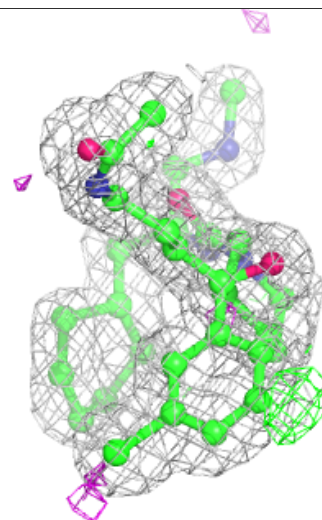
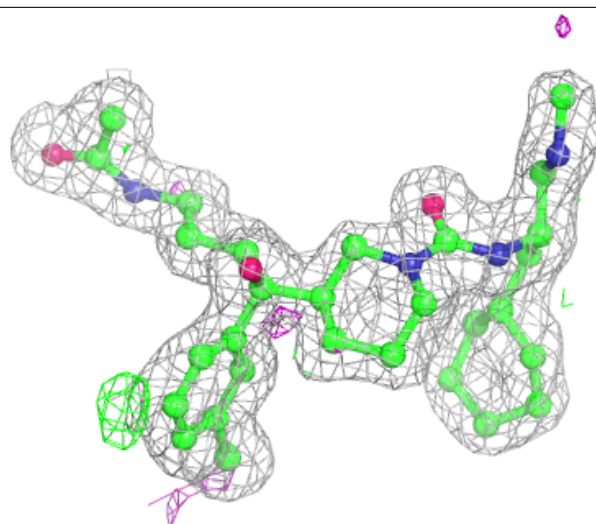
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	600	14/15	0.84	0.21	59,62,63,63	0
3	22X	A	341	36/36	0.94	0.09	12,23,31,37	0
3	22X	B	341	36/36	0.95	0.09	4,20,32,34	0
3	22X	A	400	36/36	0.96	0.13	16,20,24,34	0
3	22X	B	400	36/36	0.97	0.14	14,18,23,27	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.

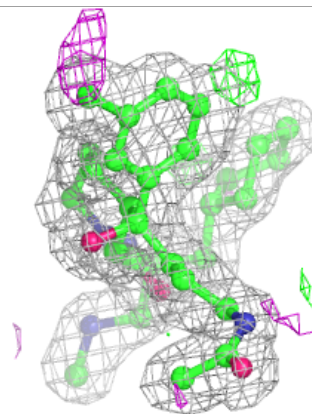
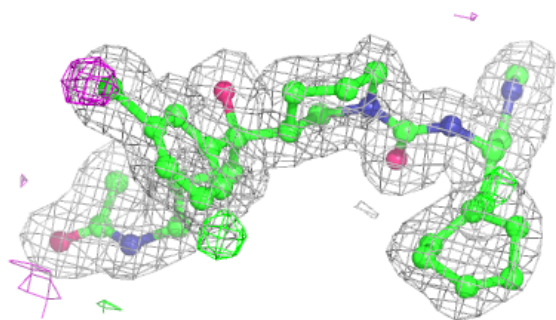
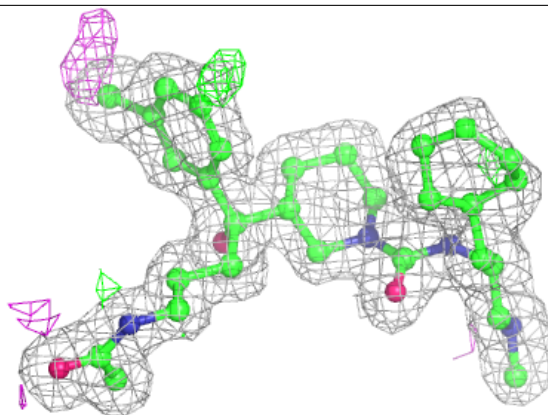
Electron density around 22X A 341:

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



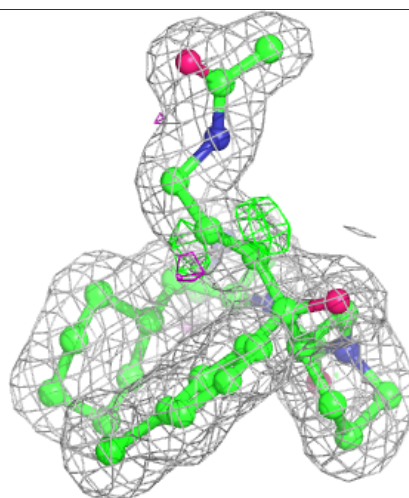
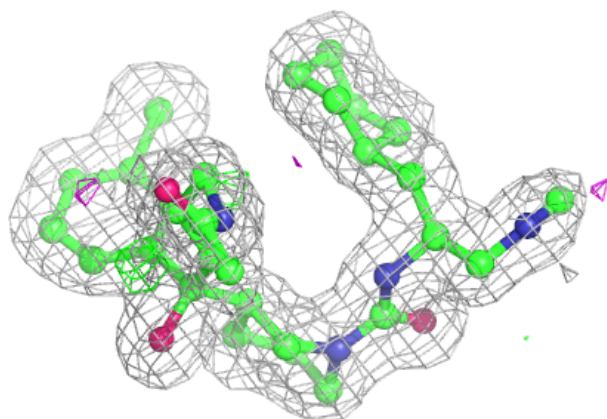
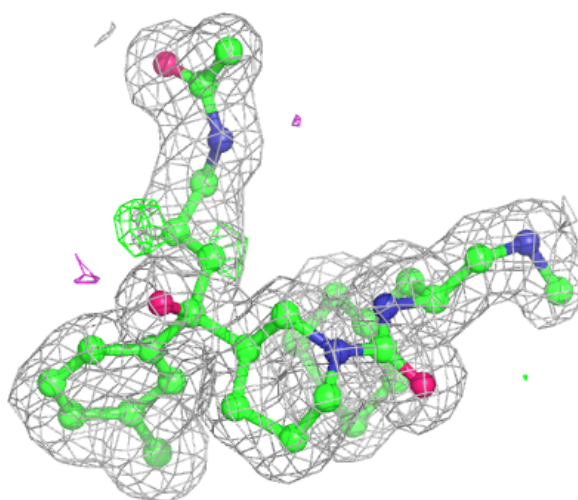
Electron density around 22X B 341:

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



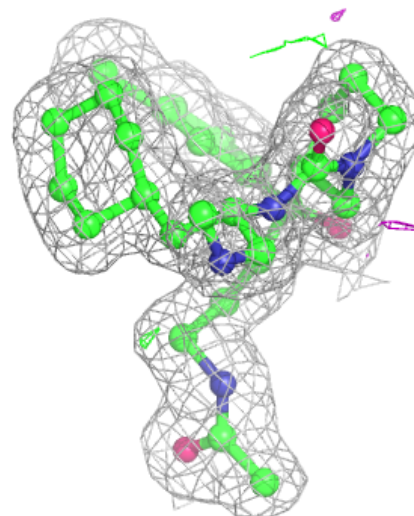
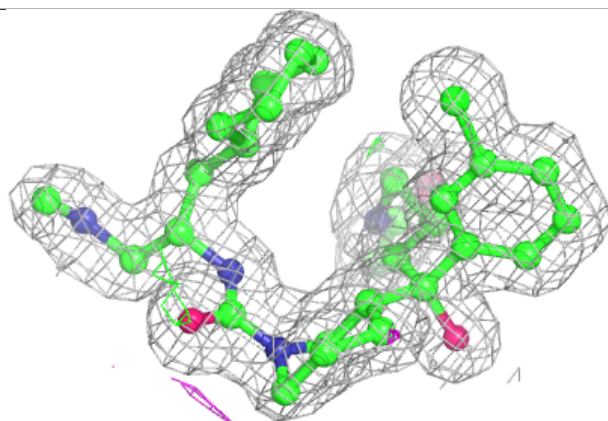
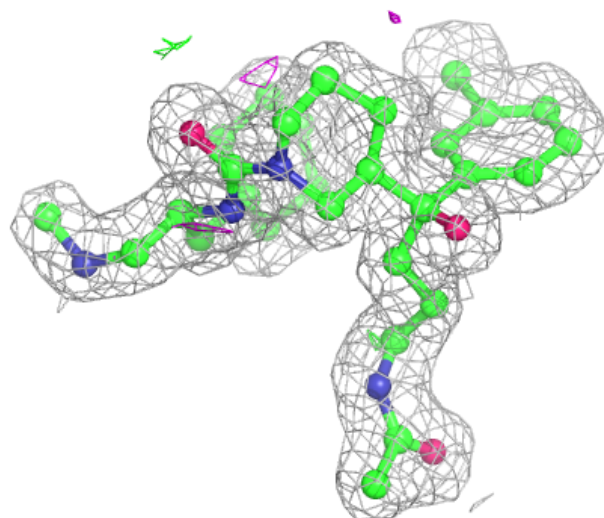
Electron density around 22X A 400:

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



Electron density around 22X B 400:

$2mF_o-DF_c$ (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.