



Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 06:11 PM JST

PDB ID : 8ZDX / pdb_00008zdx
Title : Crystal structure of MjHKU4r-CoV-1 RBD bound to hDPP4
Authors : Yang, M.; Li, Z.; Xu, Y.; Zhang, S.
Deposited on : 2024-05-03
Resolution : 2.60 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:

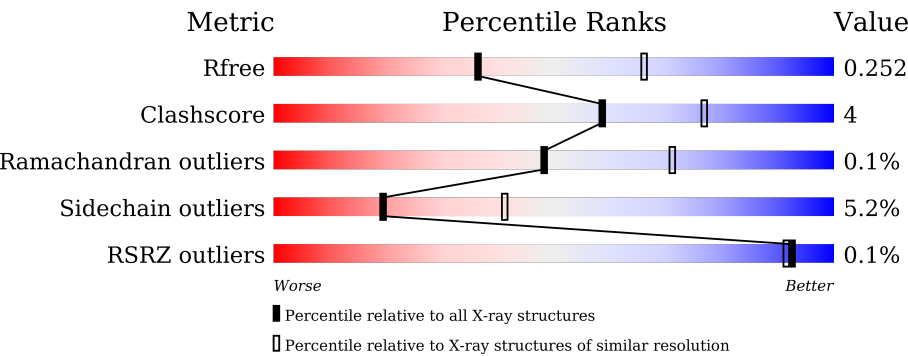
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

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 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 $\leq 5\%$. 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	729	83%15%.
1	C	729	88%12%
2	B	208	%80%17%..
2	D	208	82%16%.
3	E	3	33%33%33%
3	F	3	67%33%

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Mol	Chain	Length	Quality of chain
4	G	2	 50%50%
4	H	2	 100%
4	I	2	 50%50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15436 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 membrane form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			
1	C	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total	C	N	O	S	0	0	0
			1613	1031	261	307	14			
2	B	206	Total	C	N	O	S	0	0	0
			1597	1020	259	305	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	482	ALA	SER	conflict	UNP A0AAE8ZFM2
D	544	GLU	VAL	conflict	UNP A0AAE8ZFM2
B	482	ALA	SER	conflict	UNP A0AAE8ZFM2
B	544	GLU	VAL	conflict	UNP A0AAE8ZFM2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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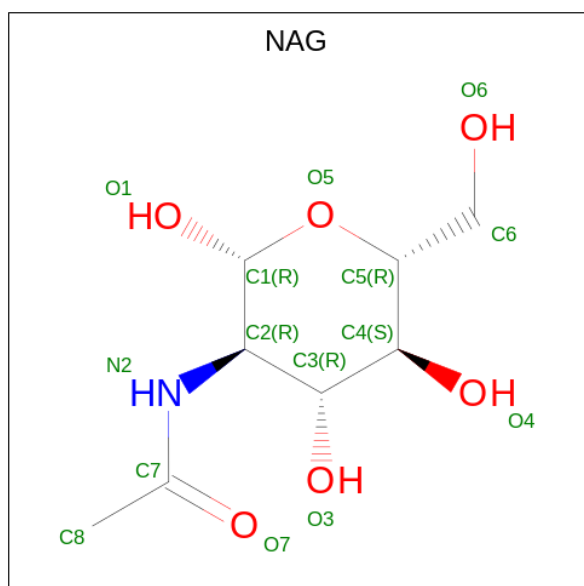
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



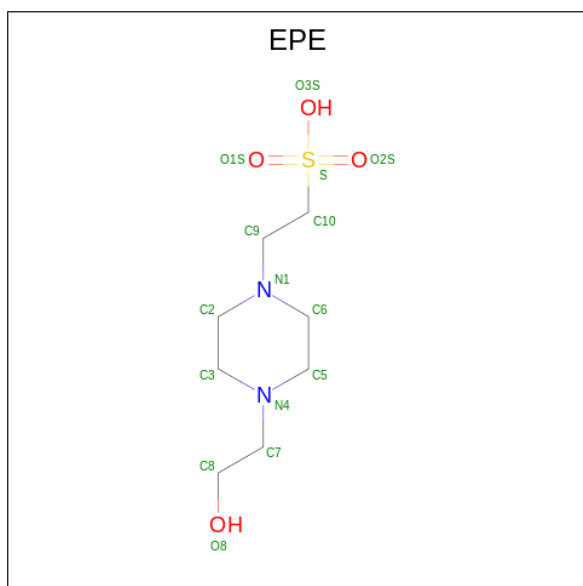
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	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 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

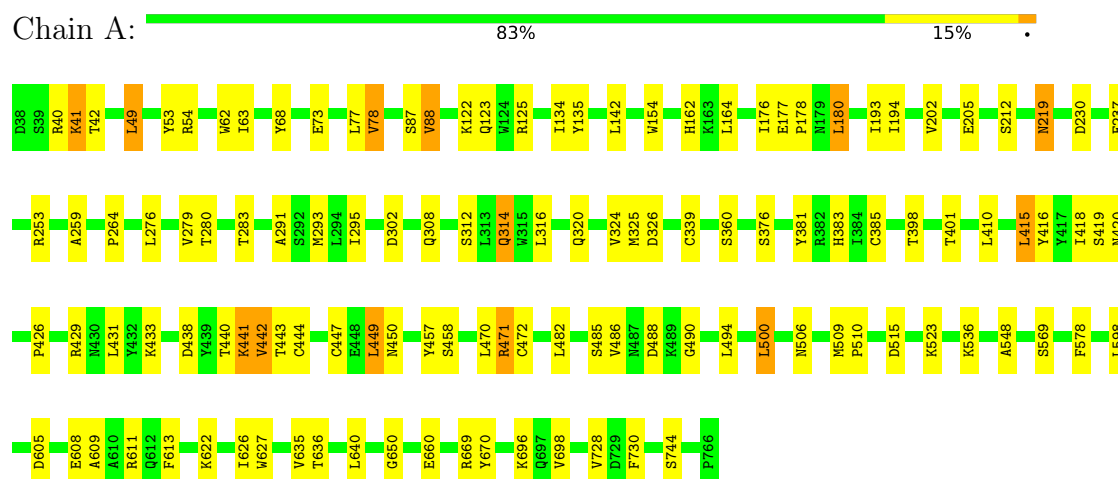
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	C	20	Total	O	0	0
			20	20		

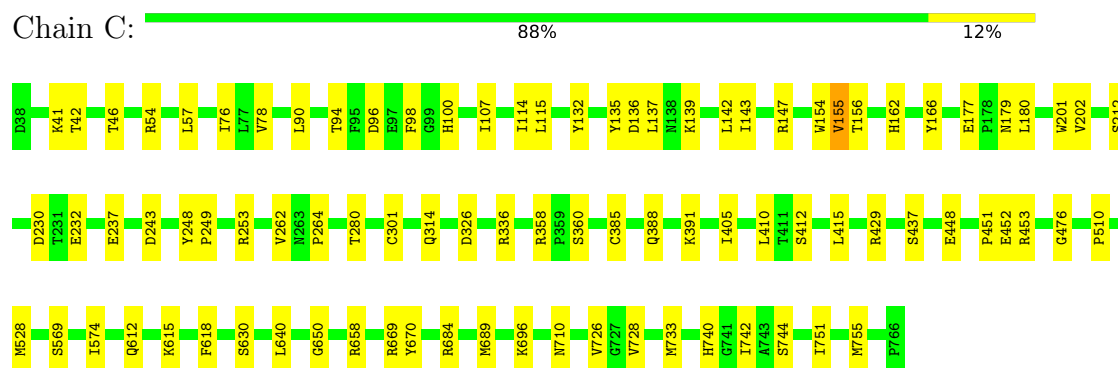
3 Residue-property plots

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.

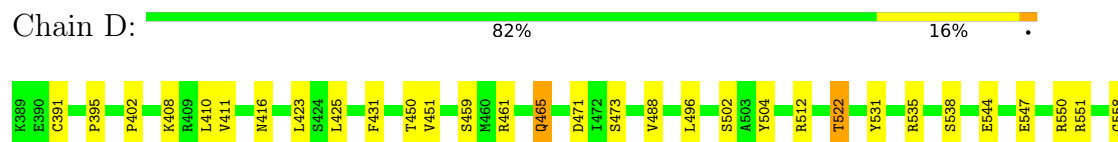
- Molecule 1: Dipeptidyl peptidase 4 membrane form



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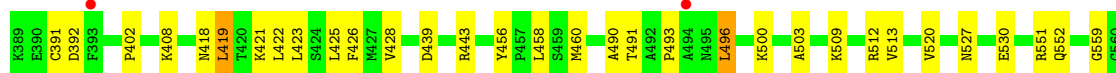
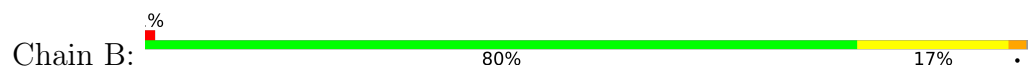


- Molecule 2: Spike glycoprotein





- Molecule 2: Spike glycoprotein



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



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



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



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



- Molecule 4: 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.98Å 121.90Å 144.66Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	19.69 – 2.60 19.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.69-2.60) 99.4 (19.69-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.59Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.208 , 0.252 0.208 , 0.252	Depositor DCC
R_{free} test set	3959 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15436	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/6143	0.28	0/8355
1	C	0.10	0/6143	0.28	0/8355
2	B	0.09	0/1637	0.28	0/2223
2	D	0.11	0/1653	0.27	0/2244
All	All	0.10	0/15576	0.28	0/21177

There are no bond length outliers.

There are no bond angle outliers.

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	5971	0	5685	58	0
1	C	5971	0	5684	39	0
2	B	1597	0	1545	18	0
2	D	1613	0	1563	16	0
3	E	39	0	34	1	0
3	F	39	0	34	1	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	42	0	39	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	C	15	0	18	1	0
7	A	3	0	0	0	0
7	C	20	0	0	0	0
All	All	15436	0	14716	130	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 4.

All (130) 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:527:ASN:HB2	2:B:530:GLU:HG3	1.63	0.80
2:B:512:ARG:HD2	2:B:559:GLY:HA3	1.69	0.74
2:D:488:VAL:HB	2:D:579:PHE:HB2	1.76	0.68
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.75	0.68
1:A:410:LEU:HD23	1:A:415:LEU:HD23	1.76	0.68
2:D:512:ARG:HB3	2:D:522:THR:HG23	1.75	0.68
2:B:491:THR:HG22	2:B:576:GLU:HG2	1.76	0.66
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.79	0.65
2:D:402:PRO:HG3	2:D:408:LYS:HG3	1.79	0.65
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.78	0.64
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.83	0.61
1:A:314:GLN:NE2	1:A:360:SER:O	2.35	0.59
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.86	0.57
2:B:551:ARG:NH1	2:B:552:GLN:O	2.38	0.57
2:B:402:PRO:HG3	2:B:408:LYS:HG3	1.86	0.57
1:C:142:LEU:HD21	1:C:147:ARG:HH21	1.68	0.57
2:D:461:ARG:O	2:D:465:GLN:NE2	2.38	0.56
1:A:125:ARG:HD2	1:A:205:GLU:OE2	2.05	0.56
1:C:115:LEU:HD11	1:C:132:TYR:HB3	1.88	0.55
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.88	0.55
3:F:2:NAG:H83	3:F:2:NAG:H3	1.89	0.55
1:C:453:ARG:HG3	1:C:476:GLY:HA3	1.89	0.55
1:A:312:SER:HB2	1:A:325:MET:HE3	1.89	0.54
1:C:388:GLN:HB2	1:C:391:LYS:HB3	1.89	0.54
1:C:448:GLU:HA	1:C:451:PRO:HG3	1.89	0.54
1:A:482:LEU:HD12	1:A:494:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASN:HD22	1:A:426:PRO:HA	1.73	0.53
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.90	0.53
1:A:696:LYS:HG2	1:A:728:VAL:HG22	1.91	0.53
1:A:383:HIS:HB3	1:A:398:THR:HB	1.90	0.53
1:C:301:CYS:O	1:C:358:ARG:NH1	2.36	0.53
1:A:295:ILE:HD13	2:B:513:VAL:HG11	1.89	0.52
1:C:155:VAL:HG13	1:C:166:TYR:HB3	1.91	0.52
1:A:135:TYR:HD1	1:A:142:LEU:HG	1.73	0.52
1:A:416:TYR:HE1	1:A:433:LYS:HD3	1.75	0.52
2:D:451:VAL:HG22	2:D:581:ILE:HG13	1.92	0.52
1:C:76:ILE:HD13	1:C:107:ILE:HD11	1.92	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.45	0.51
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.91	0.51
1:A:608:GLU:HA	1:A:611:ARG:HD3	1.90	0.51
2:B:423:LEU:HD12	2:B:428:VAL:HG11	1.93	0.51
1:A:730:PHE:CZ	1:C:733:MET:HE1	2.46	0.51
1:C:230:ASP:OD1	1:C:264:PRO:HB3	2.11	0.51
2:B:500:LYS:HG2	2:B:575:LEU:HB3	1.93	0.50
1:C:751:ILE:HG12	1:C:755:MET:HE2	1.92	0.50
1:C:232:GLU:HB2	1:C:262:VAL:HG11	1.94	0.49
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.95	0.49
2:B:503:ALA:HA	2:B:571:MET:HG2	1.95	0.48
3:E:1:NAG:H62	3:E:2:NAG:C7	2.44	0.48
1:A:509:MET:HE3	1:A:510:PRO:HD2	1.96	0.48
1:C:612:GLN:HA	1:C:615:LYS:HE3	1.95	0.48
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.96	0.47
1:C:41:LYS:HG2	1:C:42:THR:N	2.29	0.47
2:D:395:PRO:HG2	2:D:410:LEU:HD11	1.95	0.47
2:D:531:TYR:HB3	2:D:535:ARG:HD2	1.96	0.47
1:C:528:MET:HE3	1:C:574:ILE:HG21	1.97	0.47
1:A:578:PHE:HE2	1:A:605:ASP:HB3	1.79	0.47
1:C:237:GLU:HG2	1:C:253:ARG:HG3	1.97	0.47
1:C:405:ILE:HG12	1:C:429:ARG:NE	2.29	0.47
1:A:78:VAL:HG13	1:A:87:SER:HB2	1.96	0.47
1:C:90:LEU:HD12	1:C:137:LEU:HD21	1.98	0.46
1:A:429:ARG:HB2	1:A:457:TYR:H	1.80	0.46
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.98	0.46
2:B:418:ASN:ND2	2:B:421:LYS:HB2	2.31	0.46
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.98	0.46
1:C:98:PHE:C	1:C:100:HIS:H	2.23	0.46
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:504:TYR:HB2	2:D:569:LEU:HB3	1.98	0.45
2:B:493:PRO:HD2	2:B:496:LEU:HD12	1.98	0.45
2:D:402:PRO:HD3	2:D:408:LYS:HE3	1.97	0.45
1:A:279:VAL:HG23	1:A:280:THR:HG23	1.99	0.45
6:C:802:EPE:H102	6:C:802:EPE:H62	1.47	0.45
1:A:53:TYR:HB3	1:A:500:LEU:HD21	1.98	0.45
1:A:134:ILE:HD13	1:A:178:PRO:HB3	1.98	0.45
2:D:544:GLU:HG3	2:D:547:GLU:HG2	1.99	0.45
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.99	0.45
1:A:598:LEU:HD11	1:A:670:TYR:HB2	1.99	0.44
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.99	0.44
1:A:219:ASN:HB3	1:A:308:GLN:NE2	2.32	0.44
1:C:658:ARG:HB2	1:C:689:MET:HE1	2.00	0.44
1:A:441:LYS:HA	1:A:441:LYS:HD2	1.50	0.44
1:C:528:MET:HE1	1:C:618:PHE:CE1	2.53	0.44
1:A:293:MET:HE2	1:A:324:VAL:HG12	1.99	0.43
1:A:433:LYS:O	1:A:442:VAL:HA	2.19	0.43
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.87	0.43
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.99	0.43
1:C:143:ILE:HD12	1:C:179:ASN:HB3	2.00	0.43
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.54	0.43
1:A:41:LYS:HB2	1:A:41:LYS:HE2	1.70	0.43
1:A:62:TRP:CE3	1:A:68:TYR:HB3	2.53	0.43
1:A:419:SER:OG	1:A:420:ASN:N	2.52	0.43
2:B:571:MET:HE1	2:B:575:LEU:HA	2.00	0.43
1:A:449:LEU:HD22	1:A:449:LEU:HA	1.84	0.43
1:C:136:ASP:OD2	1:C:139:LYS:HE2	2.18	0.43
1:C:630:SER:HB2	1:C:740:HIS:NE2	2.34	0.43
2:B:426:PHE:HB3	2:B:490:ALA:HB1	2.01	0.43
1:C:177:GLU:HB2	1:C:180:LEU:HG	2.00	0.43
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.54	0.42
1:A:622:LYS:HD3	1:A:622:LYS:HA	1.80	0.42
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.54	0.42
2:B:456:TYR:OH	2:B:460:MET:O	2.34	0.42
1:C:314:GLN:NE2	1:C:360:SER:O	2.52	0.42
1:A:134:ILE:HG21	1:A:178:PRO:HB3	2.02	0.42
1:C:154:TRP:NE1	1:C:156:THR:OG1	2.52	0.42
2:D:416:ASN:HB3	2:D:595:MET:HG3	2.01	0.42
1:A:40:ARG:HB3	1:A:41:LYS:H	1.53	0.42
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.91	0.42
1:C:528:MET:HE1	1:C:618:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.92	0.42
1:A:122:LYS:HG2	1:A:123:GLN:N	2.34	0.42
1:C:90:LEU:HG	1:C:94:THR:HG21	2.02	0.42
1:C:336:ARG:NH1	2:D:471:ASP:OD2	2.53	0.41
2:D:550:ARG:HA	2:D:562:LEU:O	2.20	0.41
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.02	0.41
1:A:291:ALA:HB2	2:B:509:LYS:HD2	2.03	0.41
1:A:316:LEU:HD21	1:A:320:GLN:HB3	2.02	0.41
1:C:114:ILE:HG23	1:C:135:TYR:HB3	2.01	0.41
1:A:536:LYS:H	1:A:536:LYS:HD2	1.86	0.41
1:A:162:HIS:ND1	1:A:162:HIS:N	2.69	0.41
1:C:201:TRP:CZ2	1:C:710:ASN:HA	2.56	0.41
2:B:552:GLN:HG2	2:B:561:ILE:HG22	2.03	0.41
1:C:248:TYR:HA	1:C:249:PRO:HD3	1.97	0.41
2:D:431:PHE:CD1	2:D:488:VAL:HG22	2.56	0.41
2:D:512:ARG:HH12	2:D:558:GLY:HA3	1.84	0.41
1:A:609:ALA:O	1:A:613:PHE:N	2.45	0.41
2:D:425:LEU:O	2:D:496:LEU:HD11	2.21	0.41
2:B:419:LEU:HD12	2:B:419:LEU:HA	1.82	0.41
1:A:458:SER:HB3	1:A:471:ARG:HB2	2.04	0.40
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.21	0.40
1:A:418:ILE:HD13	1:A:431:LEU:HA	2.04	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	727/729 (100%)	694 (96%)	32 (4%)	1 (0%)	48	71
1	C	727/729 (100%)	690 (95%)	37 (5%)	0	100	100
2	B	204/208 (98%)	191 (94%)	12 (6%)	1 (0%)	25	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
All	All	1864/1874 (100%)	1772 (95%)	90 (5%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	591	SER
1	A	490	GLY

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	654/654 (100%)	614 (94%)	40 (6%)	15	34
1	C	654/654 (100%)	635 (97%)	19 (3%)	37	64
2	B	178/180 (99%)	166 (93%)	12 (7%)	13	29
2	D	180/180 (100%)	165 (92%)	15 (8%)	9	19
All	All	1666/1668 (100%)	1580 (95%)	86 (5%)	19	41

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	THR
1	A	49	LEU
1	A	54	ARG
1	A	63	ILE
1	A	73	GLU
1	A	78	VAL
1	A	88	VAL
1	A	176	ILE
1	A	180	LEU
1	A	202	VAL
1	A	219	ASN

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	283	THR
1	A	314	GLN
1	A	326	ASP
1	A	339	CYS
1	A	376	SER
1	A	385	CYS
1	A	415	LEU
1	A	438	ASP
1	A	440	THR
1	A	441	LYS
1	A	442	VAL
1	A	443	THR
1	A	444	CYS
1	A	447	CYS
1	A	449	LEU
1	A	450	ASN
1	A	471	ARG
1	A	472	CYS
1	A	485	SER
1	A	486	VAL
1	A	488	ASP
1	A	500	LEU
1	A	506	ASN
1	A	515	ASP
1	A	523	LYS
1	A	627	TRP
1	A	744	SER
1	C	46	THR
1	C	54	ARG
1	C	57	LEU
1	C	78	VAL
1	C	96	ASP
1	C	155	VAL
1	C	162	HIS
1	C	202	VAL
1	C	243	ASP
1	C	280	THR
1	C	326	ASP
1	C	385	CYS
1	C	412	SER
1	C	437	SER

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Mol	Chain	Res	Type
1	C	452	GLU
1	C	684	ARG
1	C	726	VAL
1	C	742	ILE
1	C	744	SER
2	D	391	CYS
2	D	411	VAL
2	D	423	LEU
2	D	450	THR
2	D	459	SER
2	D	465	GLN
2	D	473	SER
2	D	502	SER
2	D	522	THR
2	D	538	SER
2	D	551	ARG
2	D	569	LEU
2	D	588	ASP
2	D	589	THR
2	D	595	MET
2	B	391	CYS
2	B	392	ASP
2	B	419	LEU
2	B	439	ASP
2	B	443	ARG
2	B	458	LEU
2	B	496	LEU
2	B	520	VAL
2	B	561	ILE
2	B	563	VAL
2	B	571	MET
2	B	588	ASP

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	66	HIS
1	A	80	ASN
1	A	123	GLN
1	A	363	HIS
1	A	430	ASN
1	A	685	ASN

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Mol	Chain	Res	Type
1	A	757	HIS
1	C	66	HIS
1	C	72	GLN
1	C	103	ASN
1	C	227	GLN
1	C	345	HIS
1	C	369	ASN
1	C	586	GLN
1	C	595	ASN
1	C	697	GLN
1	C	749	GLN
2	D	403	GLN
2	D	429	ASN
2	D	465	GLN

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 ⓘ

12 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	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.35	0	17,19,21	0.48	0
3	NAG	E	2	3	14,14,15	0.64	1 (7%)	17,19,21	0.57	0
3	BMA	E	3	3	11,11,12	0.64	0	15,15,17	0.85	0
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	2	3	14,14,15	0.37	0	17,19,21	1.28	2 (11%)
3	BMA	F	3	3	11,11,12	0.70	0	15,15,17	1.02	0
4	NAG	G	1	1,4	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	1.01	2 (11%)
4	NAG	H	1	1,4	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	H	2	4	14,14,15	0.27	0	17,19,21	0.35	0
4	NAG	I	1	1,4	14,14,15	0.91	1 (7%)	17,19,21	0.71	1 (5%)
4	NAG	I	2	4	14,14,15	0.37	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-2.76	1.39	1.43
3	E	2	NAG	O5-C1	-2.14	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	G	2	NAG	C1-O5-C5	2.96	116.20	112.19
4	G	2	NAG	C3-C4-C5	2.27	114.29	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C4-C3-C2	2.07	114.05	111.02
3	F	2	NAG	C1-C2-N2	2.07	114.02	110.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

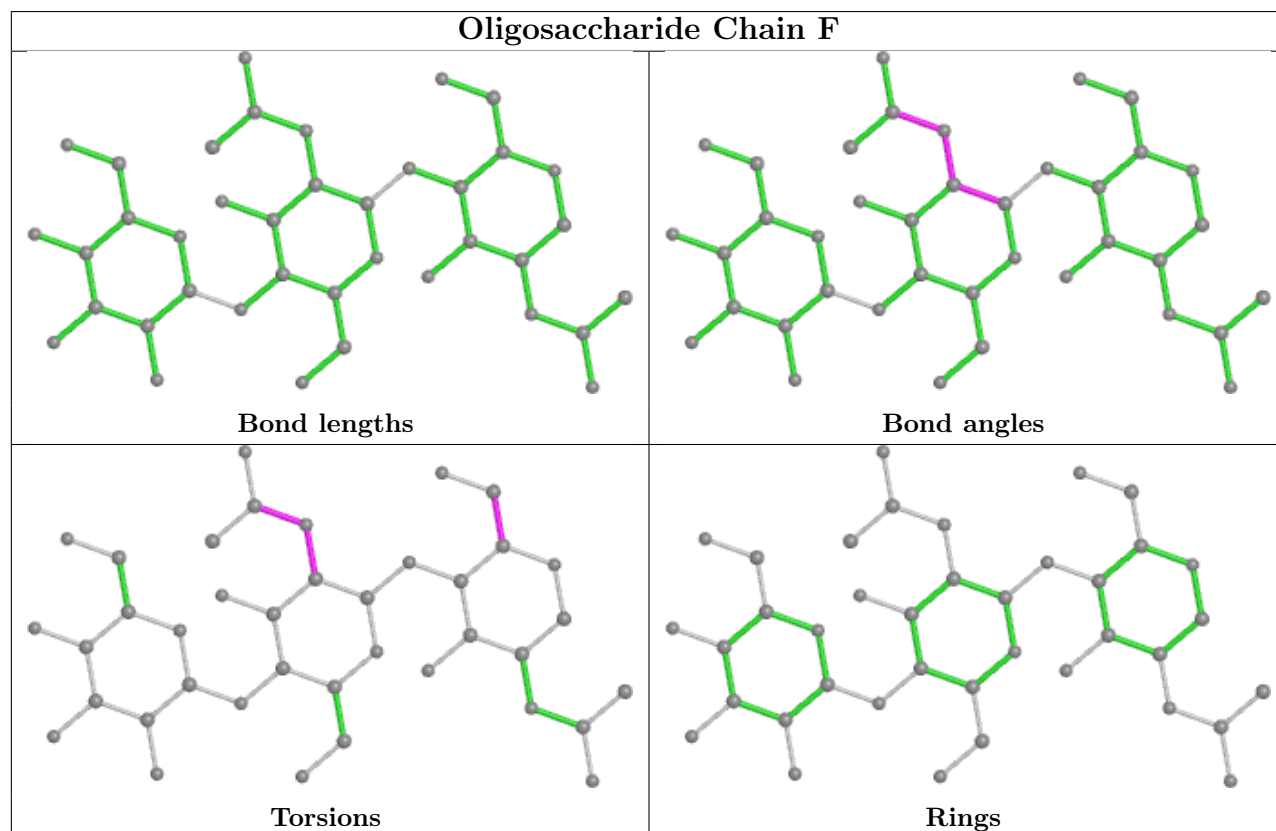
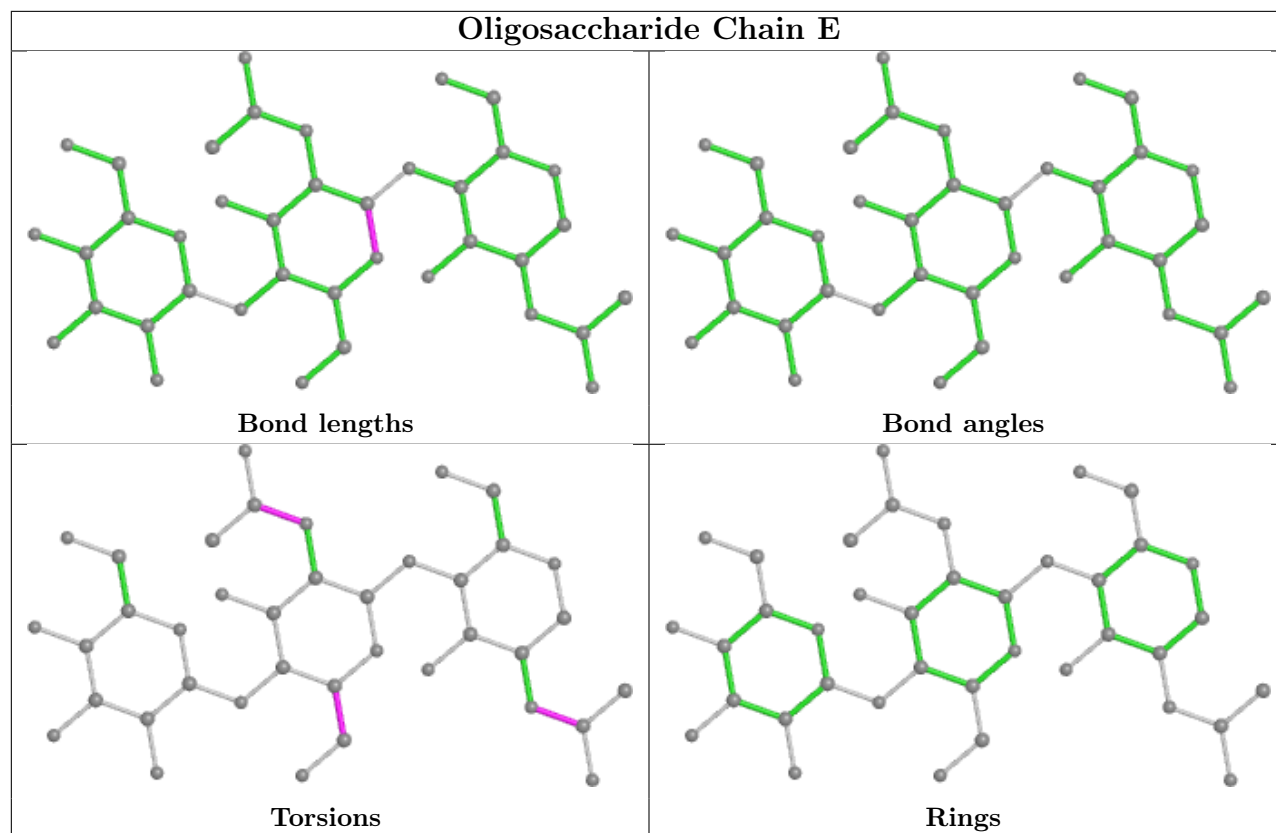
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7

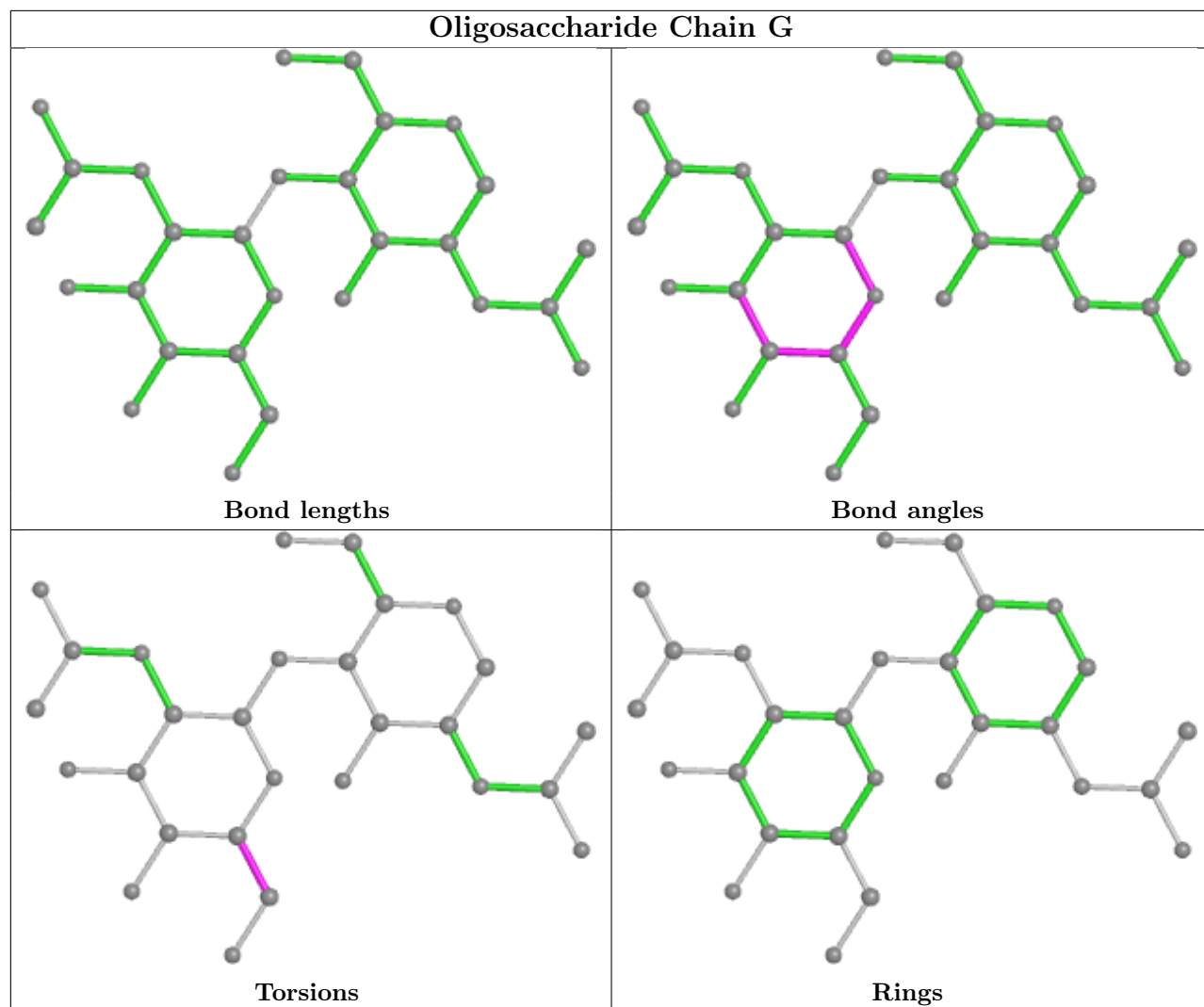
There are no ring outliers.

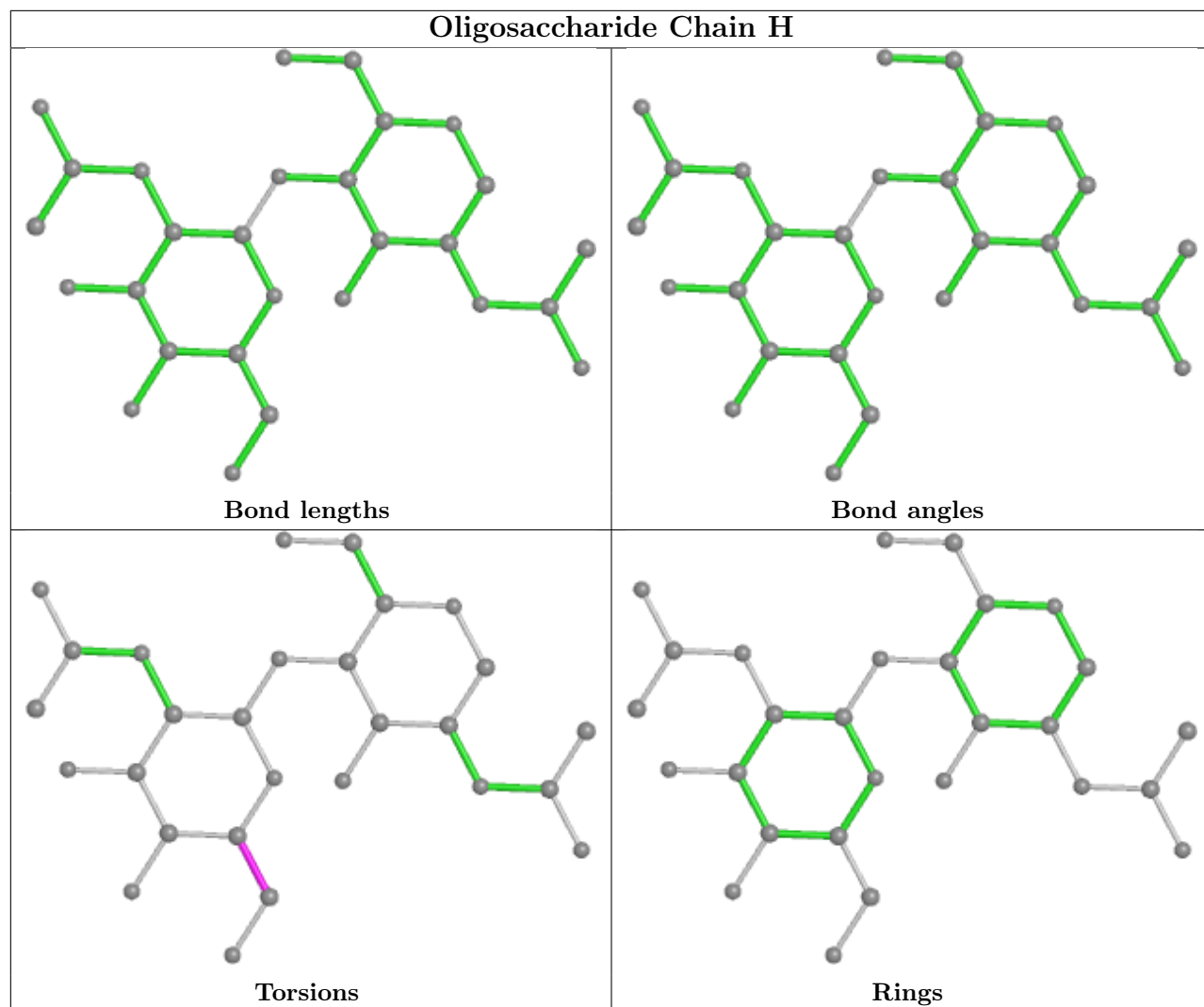
3 monomers are involved in 2 short contacts:

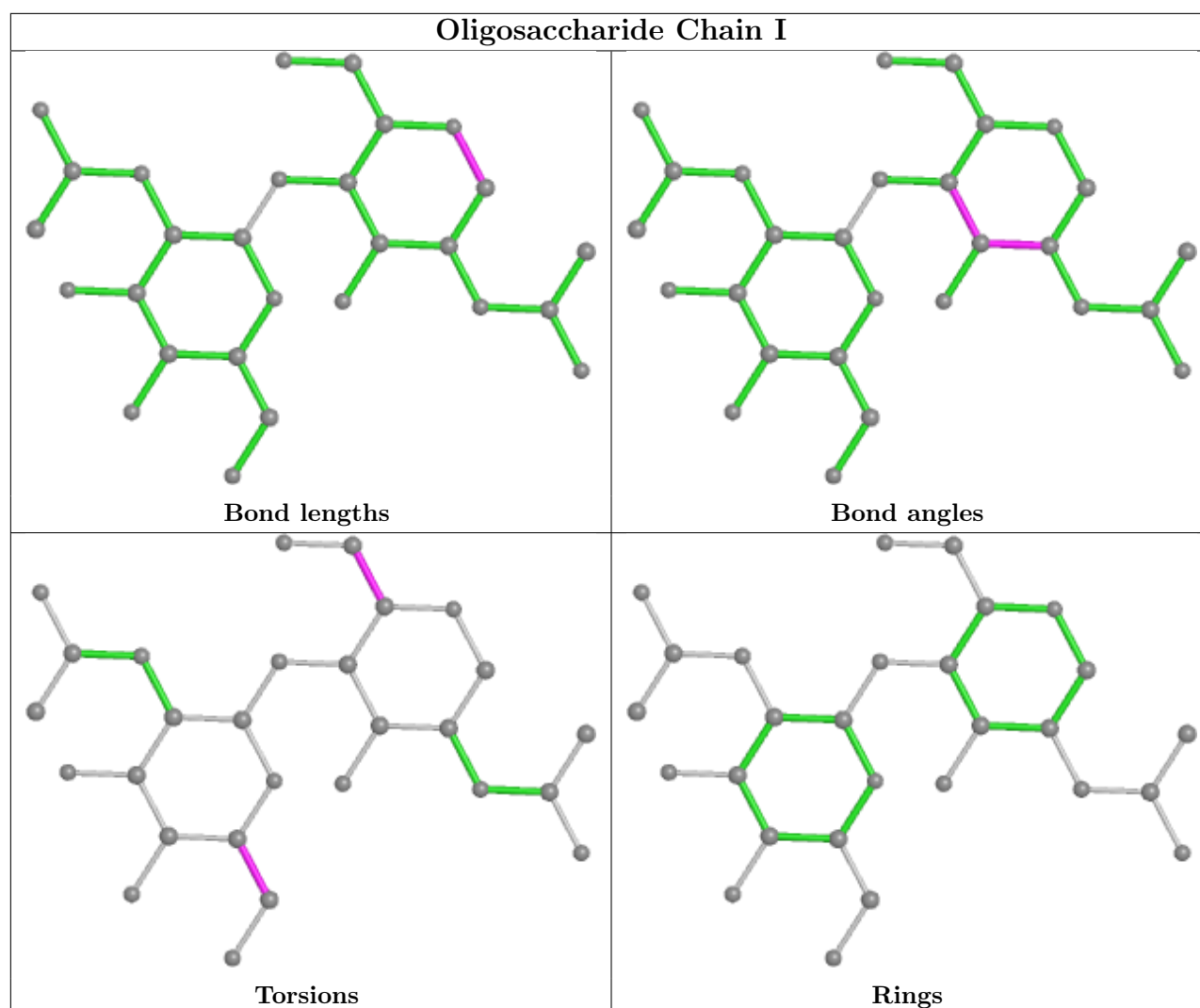
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	E	1	NAG	1	0
3	E	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
5	NAG	C	801	1	14,14,15	0.40	0	17,19,21	0.56	0
5	NAG	D	601	2	14,14,15	0.19	0	17,19,21	0.43	0
5	NAG	B	601	2	14,14,15	0.21	0	17,19,21	0.38	0
5	NAG	A	802	1	14,14,15	0.51	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	803	1	14,14,15	0.69	1 (7%)	17,19,21	0.52	0
5	NAG	A	801	1	14,14,15	0.26	0	17,19,21	0.38	0
6	EPE	C	802	-	15,15,15	1.52	2 (13%)	18,20,20	2.10	7 (38%)

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	C	801	1	-	2/6/23/26	0/1/1/1
5	NAG	D	601	2	-	4/6/23/26	0/1/1/1
5	NAG	B	601	2	-	3/6/23/26	0/1/1/1
5	NAG	A	802	1	-	1/6/23/26	0/1/1/1
5	NAG	A	803	1	-	4/6/23/26	0/1/1/1
5	NAG	A	801	1	-	1/6/23/26	0/1/1/1
6	EPE	C	802	-	-	5/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	802	EPE	C10-S	4.30	1.83	1.77
5	A	803	NAG	C1-C2	2.38	1.55	1.52
6	C	802	EPE	O2S-S	2.02	1.51	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	802	EPE	O3S-S-O2S	-4.07	101.33	111.27
6	C	802	EPE	O3S-S-C10	3.52	111.46	105.77
6	C	802	EPE	C6-N1-C2	3.49	116.69	108.83
6	C	802	EPE	O2S-S-C10	3.11	110.66	106.92
6	C	802	EPE	O1S-S-C10	3.07	110.61	106.92
6	C	802	EPE	C5-C6-N1	2.58	115.93	110.64
6	C	802	EPE	C3-C2-N1	2.45	115.66	110.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

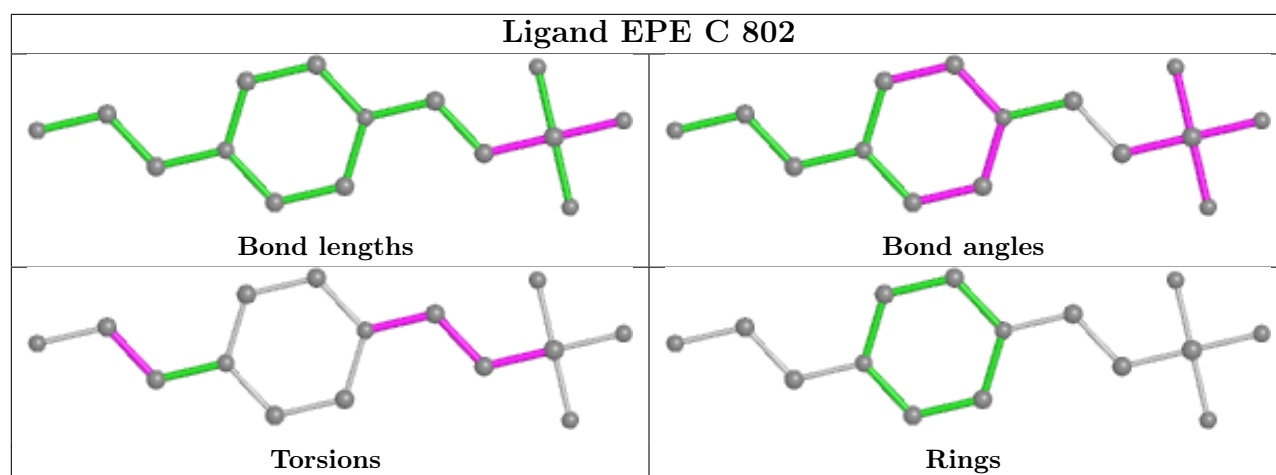
Mol	Chain	Res	Type	Atoms
6	C	802	EPE	C10-C9-N1-C6
6	C	802	EPE	S-C10-C9-N1
6	C	802	EPE	N4-C7-C8-O8
5	D	601	NAG	O5-C5-C6-O6
5	C	801	NAG	C4-C5-C6-O6
5	A	803	NAG	O5-C5-C6-O6
5	C	801	NAG	O5-C5-C6-O6
5	A	803	NAG	C4-C5-C6-O6
5	A	803	NAG	C8-C7-N2-C2
5	A	803	NAG	O7-C7-N2-C2
5	D	601	NAG	C8-C7-N2-C2
5	D	601	NAG	O7-C7-N2-C2
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
5	D	601	NAG	C4-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	A	801	NAG	O5-C5-C6-O6
6	C	802	EPE	C10-C9-N1-C2
6	C	802	EPE	C9-C10-S-O2S
5	A	802	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	802	EPE	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 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 [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(Å ²)	Q<0.9
1	A	729/729 (100%)	-0.27	0	100	100	61, 108, 145, 167	0
1	C	729/729 (100%)	-0.47	0	100	100	56, 79, 110, 152	0
2	B	206/208 (99%)	-0.14	2 (0%)	79	75	88, 119, 157, 181	0
2	D	208/208 (100%)	-0.36	0	100	100	72, 94, 133, 167	0
All	All	1872/1874 (99%)	-0.34	2 (0%)	92	91	56, 95, 143, 181	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	393	PHE	2.5
2	B	494	ALA	2.4

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.

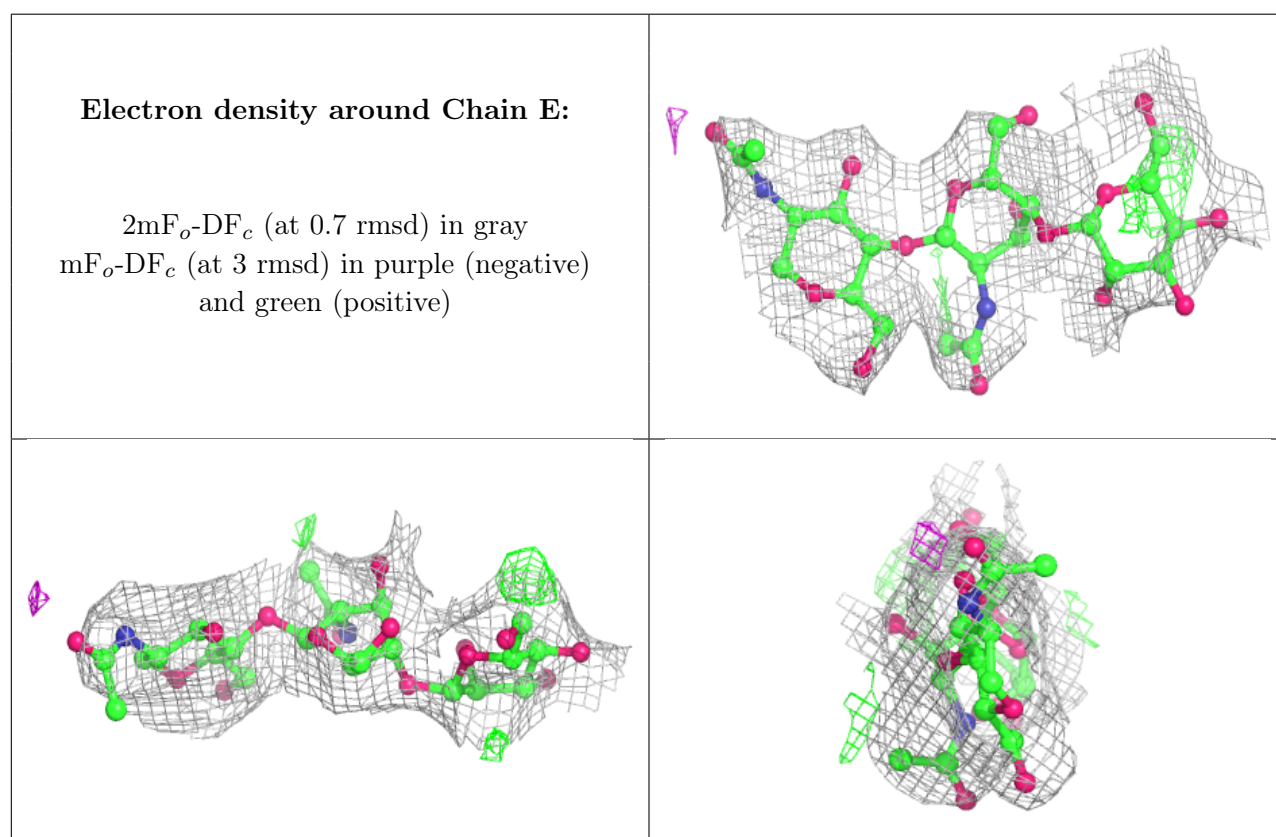
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	E	3	11/12	0.18	0.11	143,145,154,156	0
3	BMA	F	3	11/12	0.41	0.09	130,139,146,147	0
4	NAG	H	2	14/15	0.64	0.10	101,122,131,136	0
4	NAG	H	1	14/15	0.68	0.10	100,110,116,120	0
4	NAG	G	2	14/15	0.73	0.10	104,119,129,130	0

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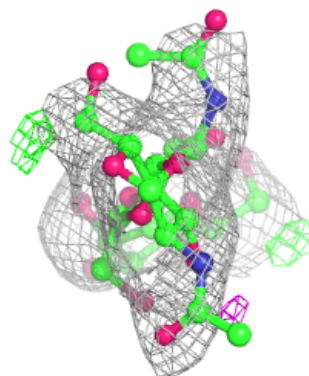
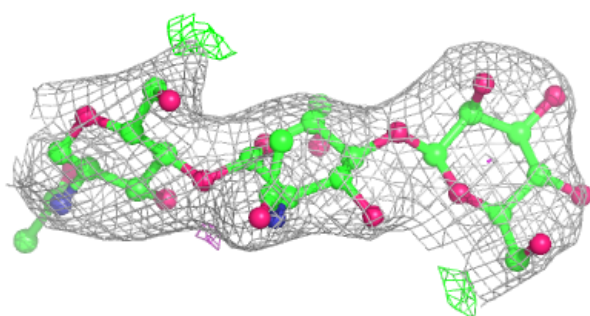
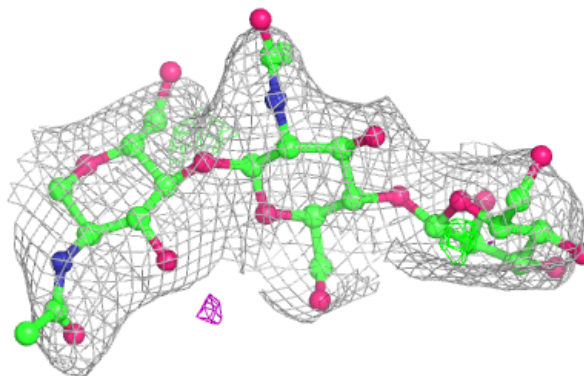
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	2	14/15	0.74	0.09	95,126,139,142	0
4	NAG	I	2	14/15	0.74	0.10	98,120,123,129	0
4	NAG	I	1	14/15	0.76	0.12	85,105,111,127	0
4	NAG	G	1	14/15	0.88	0.09	80,96,107,109	0
3	NAG	F	2	14/15	0.89	0.08	116,126,138,143	0
3	NAG	E	1	14/15	0.89	0.09	87,95,106,108	0
3	NAG	F	1	14/15	0.90	0.08	88,107,115,116	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.

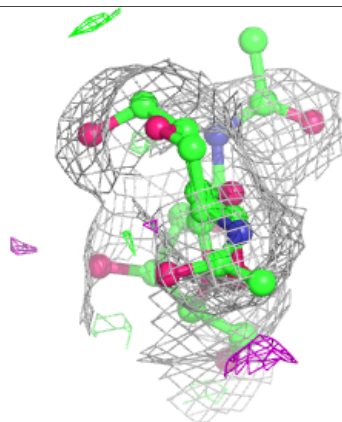
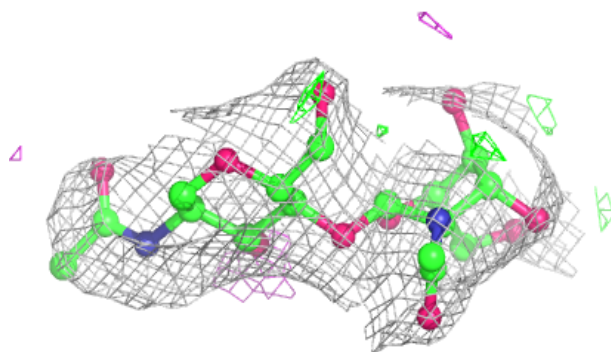
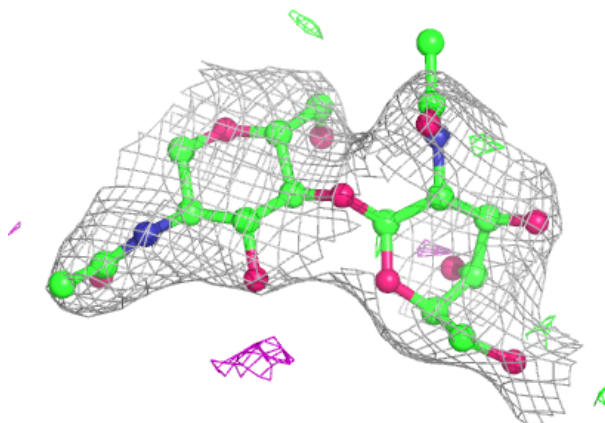


Electron density around Chain F:

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

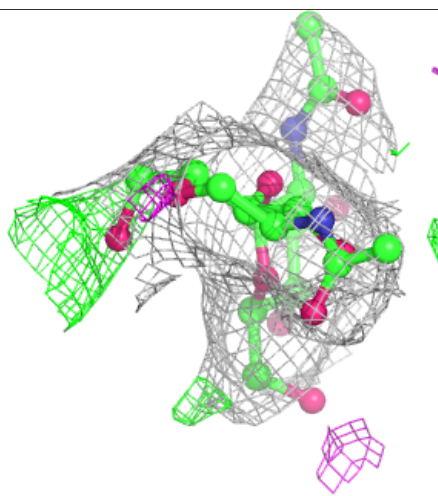
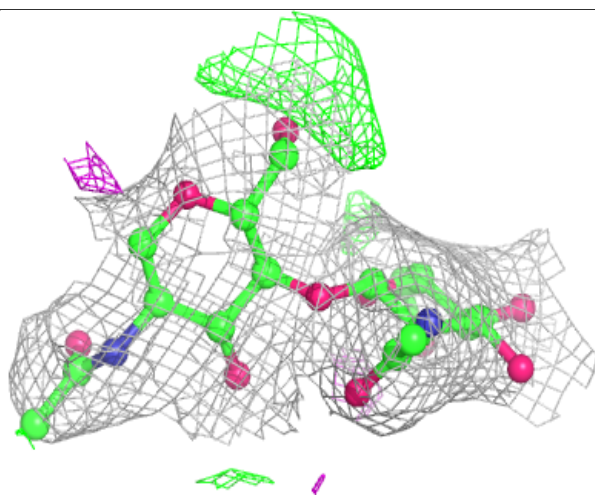
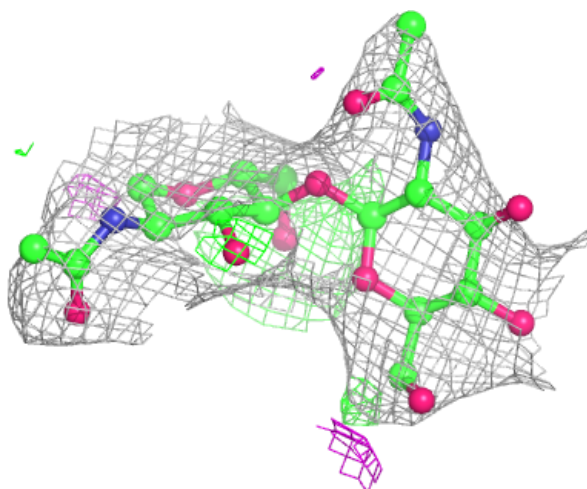
**Electron density around Chain G:**

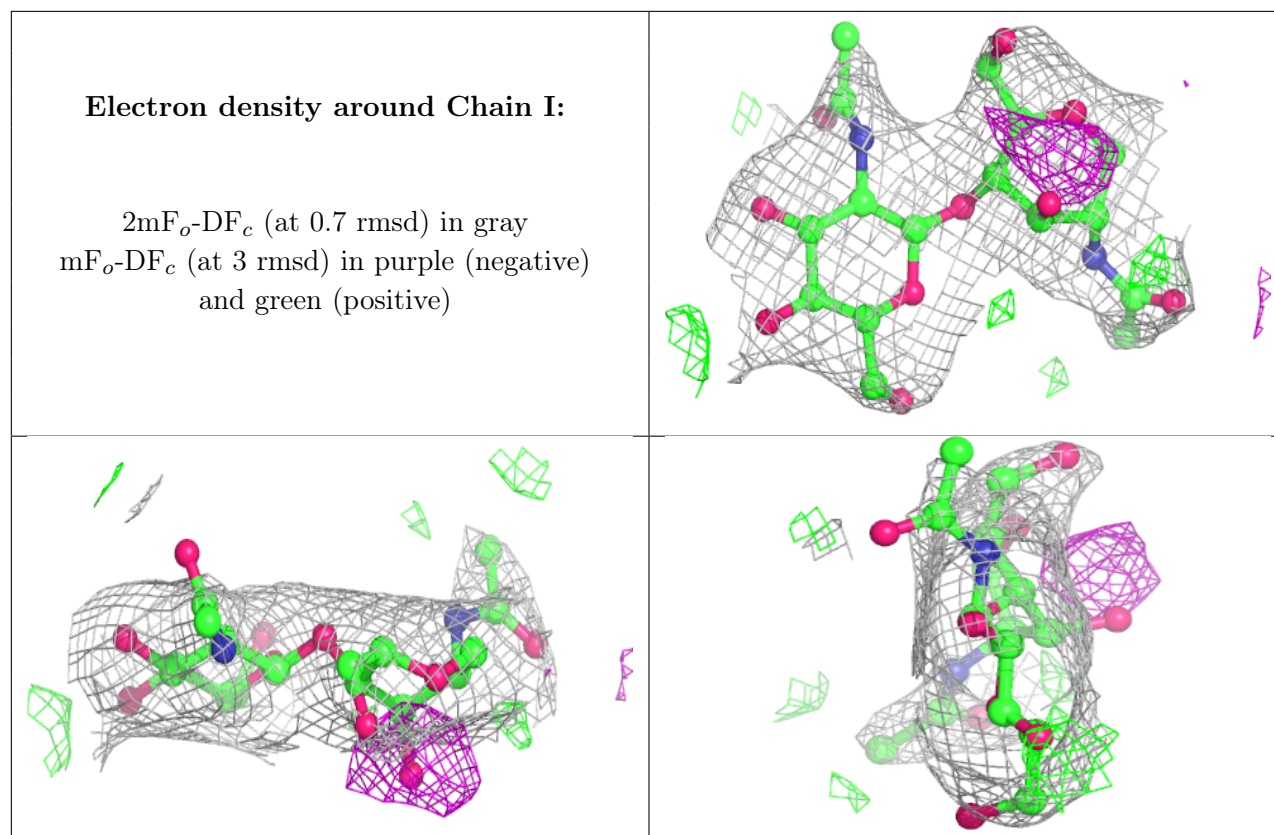
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

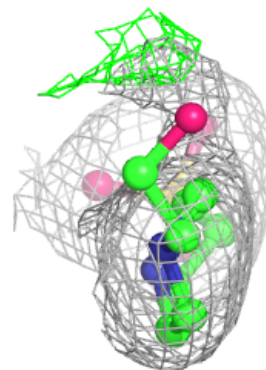
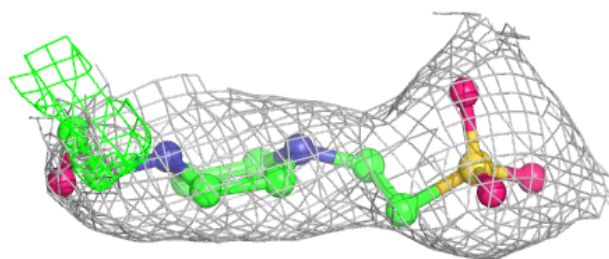
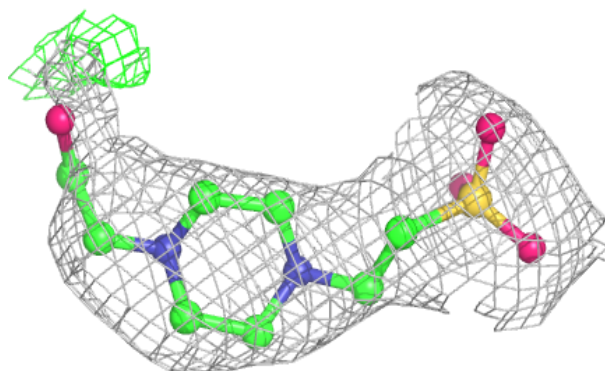
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	802	14/15	0.39	0.14	105,127,133,136	0
5	NAG	A	801	14/15	0.43	0.12	145,156,166,168	0
5	NAG	B	601	14/15	0.62	0.10	148,157,165,169	0
5	NAG	D	601	14/15	0.69	0.09	113,124,129,132	0
5	NAG	C	801	14/15	0.80	0.10	86,100,111,121	0
5	NAG	A	803	14/15	0.81	0.11	124,138,144,145	0
6	EPE	C	802	15/15	0.93	0.07	79,87,109,116	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 EPE C 802:

$2mF_o - DF_c$ (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.