



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:50 AM UTC

PDB ID : 4ZG9 / pdb_00004zg9
Title : Structural basis for inhibition of human autotaxin by four novel compounds
Authors : Stein, A.J.; Bain, G.; Hutchinson, J.H.; Evans, J.F.
Deposited on : 2015-04-22
Resolution : 2.95 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

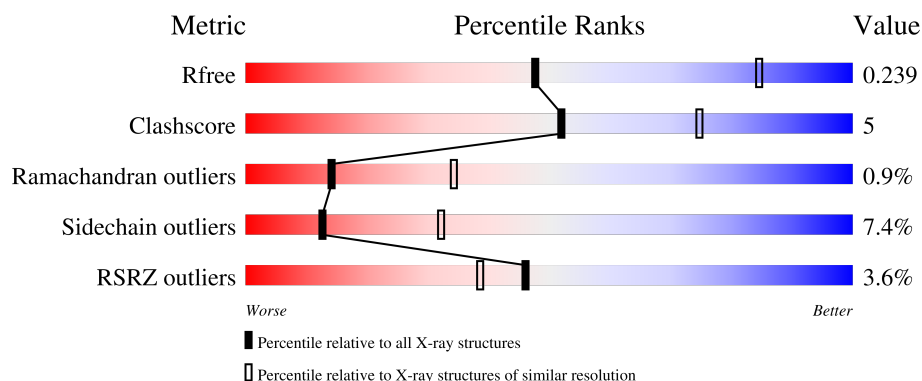
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

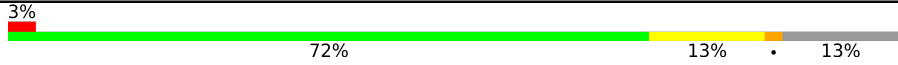
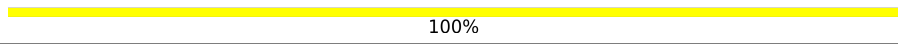
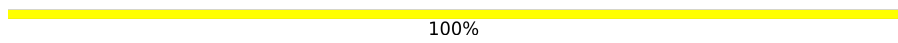
The reported resolution of this entry is 2.95 Å.

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	863	 3% 72% 13% • 13%
1	B	863	 3% 74% 12% • 11%
2	C	2	 100%
3	D	3	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12241 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

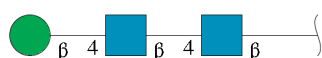
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	2	0
			5932	3783	1010	1093	46			
1	B	764	Total	C	N	O	S	0	0	0
			6045	3851	1029	1118	47			

- 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 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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

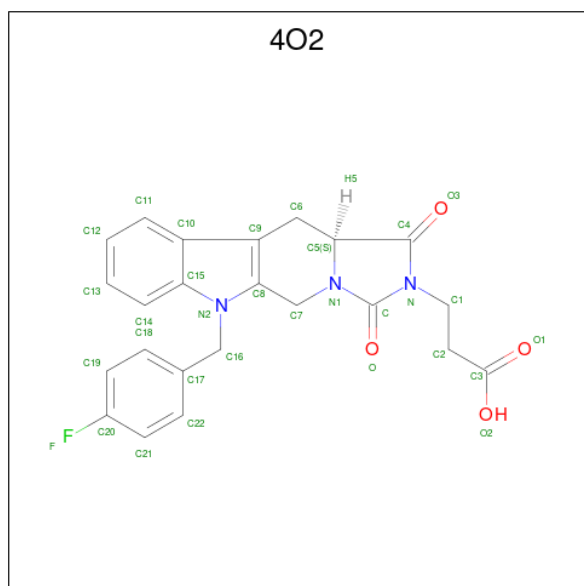
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		
6	B	2	Total	Na	0	0
			2	2		

- Molecule 7 is 3-[(11aS)-6-(4-fluorobenzyl)-1,3-dioxo-5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]pyrido[3,4-b]indol-2(3H)-yl]propanoic acid (CCD ID: 4O2) (formula: C₂₃H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			31	23	1	3	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			31	23	1	3	4		
7	B	1	Total	C	F	N	O	0	0
			31	23	1	3	4		
7	B	1	Total	C	F	N	O	0	0
			31	23	1	3	4		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

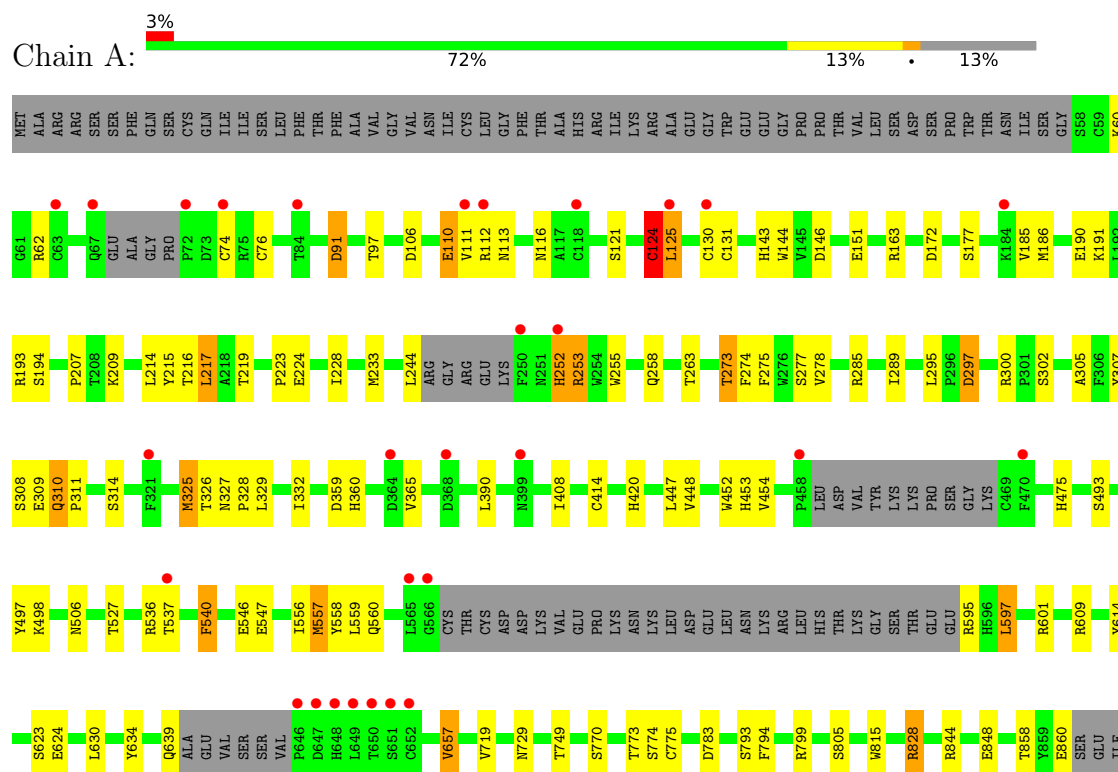
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	19	Total	O	0	0
			19	19		
9	B	32	Total	O	0	0
			32	32		

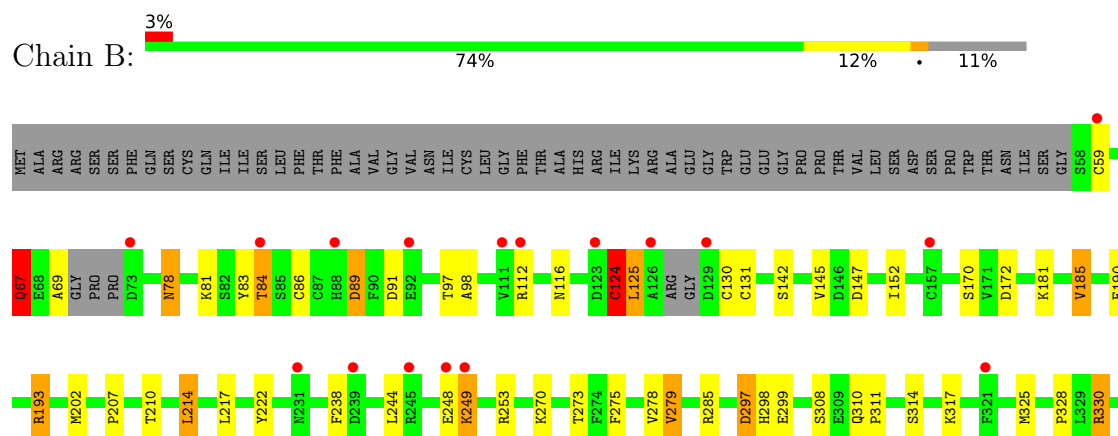
3 Residue-property plots [i](#)

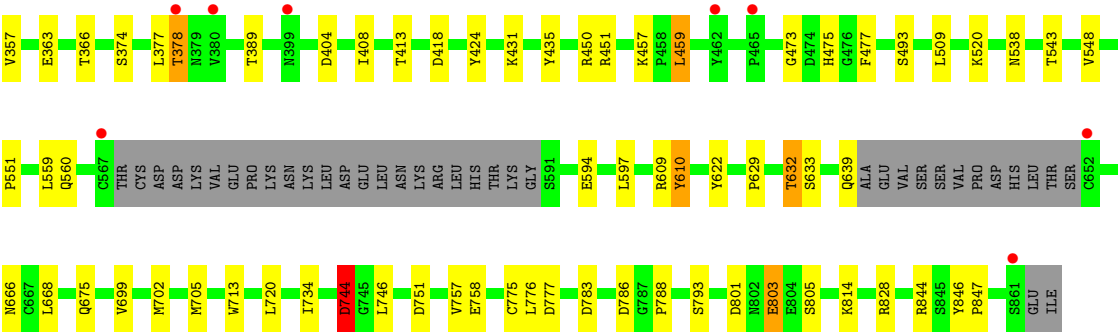
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 100%

MAG1
MAG2
BNA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.46Å 209.99Å 188.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.95 43.86 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.86-2.95) 99.3 (43.86-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.244 0.181 , 0.239	Depositor DCC
R_{free} test set	2752 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12241	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: BMA, NAG, NA, ZN, CA, 4O2, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/6113	0.97	6/8323 (0.1%)
1	B	0.79	0/6218	0.97	12/8456 (0.1%)
All	All	0.80	0/12331	0.97	18/16779 (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	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	719	VAL	N-CA-C	7.28	117.82	111.56
1	B	744	ASP	CB-CA-C	-6.38	100.19	110.79
1	B	720	LEU	N-CA-C	6.20	118.03	111.28
1	B	509	LEU	N-CA-C	6.03	117.85	111.28
1	B	222	TYR	CA-C-N	-5.99	112.69	119.28
1	B	222	TYR	C-N-CA	-5.99	112.69	119.28
1	B	548	VAL	N-CA-C	-5.96	107.08	111.90
1	B	238	PHE	N-CA-C	-5.83	102.31	110.35
1	B	249	LYS	N-CA-C	5.75	117.67	108.41
1	B	279	VAL	CB-CA-C	-5.41	104.95	112.04
1	B	610	TYR	N-CA-C	5.17	117.04	109.24
1	A	300	ARG	N-CA-C	5.14	117.01	109.71
1	A	116	ASN	N-CA-C	5.09	117.43	110.55
1	B	803	GLU	N-CA-C	-5.09	106.33	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-C-N	5.08	124.97	119.85
1	A	295	LEU	C-N-CA	5.08	124.97	119.85
1	A	634	TYR	N-CA-C	5.07	116.64	108.32
1	B	67	GLN	N-CA-C	5.03	117.19	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	TYR	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	5932	0	5534	61	0
1	B	6045	0	5674	56	0
2	C	28	0	25	0	0
3	D	39	0	34	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	62	0	38	4	0
7	B	62	0	38	4	0
8	A	8	0	12	0	0
8	B	4	0	5	0	0
9	A	19	0	0	1	0
9	B	32	0	0	1	0
All	All	12241	0	11360	121	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 5.

All (121) 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:124:CYS:SG	1:B:125:LEU:N	2.53	0.82
7:A:909:4O2:H9	7:A:909:4O2:H15	1.67	0.77
1:A:121:SER:O	1:A:124:CYS:HB3	1.85	0.77
1:B:639:GLN:OE1	1:B:639:GLN:N	2.19	0.75
1:B:83:TYR:OH	1:B:249:LYS:HG2	1.90	0.72
7:B:909:4O2:O3	7:B:909:4O2:H4	1.89	0.71
1:A:844:ARG:HD3	1:A:848:GLU:OE2	1.93	0.69
1:B:378:THR:HA	9:B:1015:HOH:O	1.93	0.68
1:A:310:GLN:HE22	1:A:314:SER:H	1.43	0.66
1:A:110:GLU:HB3	1:A:121:SER:HA	1.75	0.66
1:B:297:ASP:N	1:B:297:ASP:OD1	2.29	0.65
1:B:457:LYS:HD3	1:B:459:LEU:HD21	1.79	0.64
1:A:190:GLU:OE2	1:A:193:ARG:NH1	2.31	0.64
1:A:62:ARG:NH2	1:A:76:CYS:SG	2.71	0.63
1:B:185:VAL:HG13	1:B:330:ARG:HG2	1.80	0.62
1:B:83:TYR:C	1:B:84:THR:OG1	2.40	0.60
1:A:365:VAL:HG11	1:A:453:HIS:CD2	2.37	0.60
1:B:413:THR:HG21	1:B:803:GLU:HG3	1.84	0.60
1:B:81:LYS:HG2	1:B:86:CYS:SG	2.42	0.59
1:B:83:TYR:O	1:B:84:THR:OG1	2.18	0.59
1:B:325:MET:O	1:B:328:PRO:HD2	2.03	0.59
1:B:744:ASP:HB3	1:B:746:LEU:H	1.66	0.58
1:B:632:THR:O	1:B:734:ILE:HA	2.03	0.58
1:B:78:ASN:C	1:B:78:ASN:HD22	2.11	0.58
1:A:110:GLU:HB3	1:A:121:SER:CA	2.35	0.56
1:A:609:ARG:HD2	1:A:624:GLU:OE1	2.05	0.56
1:B:98:ALA:HB3	1:B:116:ASN:HA	1.88	0.56
1:A:310:GLN:HE21	1:A:310:GLN:HA	1.72	0.55
1:A:314:SER:C	1:A:325:MET:HE1	2.31	0.54
1:B:314:SER:CB	1:B:325:MET:HE1	2.37	0.54
1:B:78:ASN:C	1:B:78:ASN:ND2	2.64	0.54
1:A:297:ASP:N	1:A:297:ASP:OD1	2.41	0.53
1:A:255:TRP:CH2	7:A:909:4O2:H16	2.43	0.53
1:B:363:GLU:O	1:B:473:GLY:HA2	2.08	0.52
1:B:325:MET:C	1:B:328:PRO:HD2	2.34	0.52
1:A:497:TYR:CE2	1:A:498:LYS:HD2	2.45	0.52
1:B:622:TYR:HA	1:B:629:PRO:HA	1.92	0.51
1:B:202:MET:HE1	1:B:357:VAL:CG2	2.41	0.51
1:A:124:CYS:SG	1:A:125:LEU:N	2.84	0.51
1:A:310:GLN:NE2	1:A:314:SER:H	2.07	0.51
1:B:210:THR:HG22	1:B:214:LEU:HD22	1.93	0.51
1:A:91:ASP:N	1:A:91:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:HA	1:A:305:ALA:HB3	1.91	0.50
1:A:172:ASP:OD2	1:A:307:TYR:OH	2.30	0.49
1:A:151:GLU:HA	1:A:497:TYR:CD1	2.47	0.49
1:B:67:GLN:HE22	1:B:69:ALA:HB2	1.76	0.49
1:A:143:HIS:HB2	1:A:146:ASP:OD2	2.11	0.49
1:A:163:ARG:NH1	1:A:302:SER:OG	2.45	0.49
1:A:614:TYR:C	1:A:614:TYR:CD1	2.91	0.49
1:A:274:PHE:O	7:A:908:4O2:H17	2.13	0.48
1:B:308:SER:OG	1:B:310:GLN:O	2.28	0.48
1:B:78:ASN:OD1	1:B:273:THR:HG21	2.13	0.48
1:B:801:ASP:OD1	1:B:803:GLU:HB2	2.14	0.48
1:A:497:TYR:CZ	1:A:498:LYS:HD2	2.49	0.48
1:B:298:HIS:CE1	1:B:299:GLU:OE1	2.66	0.48
1:B:705:MET:HE1	1:B:713:TRP:CE2	2.49	0.48
1:A:207:PRO:HB2	1:A:209:LYS:HG2	1.97	0.47
1:B:207:PRO:HD3	1:B:435:TYR:CE1	2.49	0.47
1:B:89:ASP:OD1	1:B:89:ASP:N	2.47	0.47
1:B:551:PRO:HB3	1:B:610:TYR:CE2	2.50	0.47
1:B:81:LYS:NZ	1:B:91:ASP:OD1	2.41	0.47
1:B:450:ARG:O	1:B:451:ARG:HB2	2.14	0.47
1:B:363:GLU:OE2	1:B:450:ARG:NH2	2.47	0.47
1:A:172:ASP:O	1:A:311:PRO:HD2	2.14	0.47
1:A:217:LEU:HD13	1:A:506:ASN:HB2	1.97	0.47
1:A:558:TYR:O	1:A:657:VAL:HG22	2.14	0.47
1:B:275:PHE:HA	7:B:909:4O2:O	2.15	0.46
1:A:536:ARG:HG2	1:A:537:THR:HG23	1.98	0.46
1:B:310:GLN:OE1	1:B:311:PRO:HA	2.15	0.46
1:A:556:ILE:HG23	1:A:657:VAL:CG1	2.45	0.46
7:B:910:4O2:O3	7:B:910:4O2:H4	2.15	0.46
1:B:202:MET:HE1	1:B:357:VAL:HG23	1.98	0.46
1:A:258:GLN:OE1	1:A:263:THR:HA	2.16	0.45
1:A:360:HIS:CE1	1:A:475:HIS:CE1	3.05	0.45
1:A:216:THR:O	1:A:217:LEU:C	2.59	0.44
1:A:308:SER:OG	1:A:332:ILE:HD11	2.17	0.44
1:A:106:ASP:OD1	1:A:106:ASP:N	2.49	0.44
1:A:770:SER:HB2	1:A:794:PHE:CZ	2.53	0.44
1:B:757:VAL:O	1:B:758:GLU:C	2.61	0.44
1:A:215:TYR:O	1:A:219:THR:HG23	2.18	0.44
1:B:431:LYS:HA	1:B:431:LYS:HD2	1.76	0.44
1:A:151:GLU:HA	1:A:497:TYR:CE1	2.53	0.43
7:A:909:4O2:H15	7:A:909:4O2:C7	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:O	1:A:113:ASN:N	2.42	0.43
1:B:776:LEU:CD2	1:B:788:PRO:HB2	2.49	0.43
1:B:314:SER:C	1:B:325:MET:HE1	2.44	0.43
1:A:223:PRO:O	1:A:224:GLU:C	2.60	0.43
1:B:97:THR:O	1:B:97:THR:HG22	2.17	0.43
1:B:666:ASN:OD1	1:B:668:LEU:HB3	2.19	0.43
1:B:83:TYR:HE2	1:B:249:LYS:HD3	1.84	0.43
1:B:314:SER:HB3	1:B:325:MET:HE1	2.00	0.43
1:B:777:ASP:OD1	1:B:777:ASP:C	2.62	0.43
1:A:327:ASN:HB2	1:A:328:PRO:HD3	2.00	0.43
1:B:170:SER:HA	1:B:357:VAL:O	2.18	0.43
1:B:699:VAL:HG23	1:B:702:MET:HE2	2.01	0.42
1:A:359:ASP:OD1	1:A:360:HIS:N	2.53	0.42
1:A:144:TRP:CH2	1:A:191:LYS:HG2	2.55	0.42
1:B:190:GLU:OE2	1:B:193:ARG:NH1	2.53	0.42
1:A:527:THR:OG1	1:A:828:ARG:HD3	2.19	0.42
1:A:557:MET:HB3	1:A:558:TYR:CD1	2.55	0.42
1:B:142:SER:OG	1:B:147:ASP:OD1	2.35	0.42
1:A:228:ILE:HG23	1:A:244:LEU:HD11	2.02	0.41
1:A:448:VAL:HG22	1:A:454:VAL:HG21	2.02	0.41
1:A:595:ARG:NH1	1:A:783:ASP:OD2	2.53	0.41
1:A:597:LEU:HD11	1:A:601:ARG:HB3	2.01	0.41
1:A:186:MET:SD	1:A:329:LEU:HB3	2.60	0.41
1:A:252[B]:HIS:CE1	1:A:253:ARG:HD3	2.55	0.41
1:A:273:THR:HB	1:A:275:PHE:H	1.86	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.92	0.41
1:A:285:ARG:O	1:A:289:ILE:HG13	2.21	0.41
1:A:540:PHE:HA	9:A:1007:HOH:O	2.21	0.41
1:A:623:SER:HB2	1:A:630:LEU:HD21	2.03	0.41
1:B:389:THR:HG22	1:B:477:PHE:CZ	2.56	0.41
1:A:314:SER:HB3	1:A:325:MET:HE1	2.03	0.40
1:B:285:ARG:NH2	7:B:909:4O2:O1	2.54	0.40
1:B:404:ASP:O	1:B:408:ILE:HG12	2.21	0.40
1:A:325:MET:C	1:A:328:PRO:HD2	2.46	0.40
1:A:420:HIS:CD2	1:A:452:TRP:CZ2	3.09	0.40
1:B:83:TYR:CE2	1:B:249:LYS:HD3	2.57	0.40
1:B:846:TYR:N	1:B:847:PRO:CD	2.85	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	740/863 (86%)	682 (92%)	52 (7%)	6 (1%)	16	37
1	B	754/863 (87%)	695 (92%)	52 (7%)	7 (1%)	14	34
All	All	1494/1726 (87%)	1377 (92%)	104 (7%)	13 (1%)	14	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	124	CYS
1	B	78	ASN
1	A	414	CYS
1	B	124	CYS
1	B	181	LYS
1	B	248	GLU
1	B	374	SER
1	A	112	ARG
1	B	112	ARG
1	B	751	ASP
1	A	815	TRP
1	A	729	ASN

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	642/780 (82%)	595 (93%)	47 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	656/780 (84%)	606 (92%)	50 (8%)	12	31
All	All	1298/1560 (83%)	1201 (92%)	97 (8%)	13	31

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	CYS
1	A	91	ASP
1	A	97	THR
1	A	110	GLU
1	A	124	CYS
1	A	125	LEU
1	A	130	CYS
1	A	131	CYS
1	A	177	SER
1	A	185	VAL
1	A	194	SER
1	A	217	LEU
1	A	233	MET
1	A	252[A]	HIS
1	A	252[B]	HIS
1	A	253	ARG
1	A	273	THR
1	A	277	SER
1	A	278	VAL
1	A	297	ASP
1	A	309	GLU
1	A	310	GLN
1	A	325	MET
1	A	326	THR
1	A	390	LEU
1	A	408	ILE
1	A	447	LEU
1	A	493	SER
1	A	540	PHE
1	A	546	GLU
1	A	547	GLU
1	A	557	MET
1	A	559	LEU
1	A	560	GLN
1	A	597	LEU
1	A	639	GLN

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Mol	Chain	Res	Type
1	A	657	VAL
1	A	749	THR
1	A	773	THR
1	A	774	SER
1	A	775	CYS
1	A	793	SER
1	A	799	ARG
1	A	805	SER
1	A	828	ARG
1	A	858	THR
1	A	860	GLU
1	B	59	CYS
1	B	67	GLN
1	B	84	THR
1	B	89	ASP
1	B	124	CYS
1	B	125	LEU
1	B	130	CYS
1	B	131	CYS
1	B	145	VAL
1	B	152	ILE
1	B	172	ASP
1	B	185	VAL
1	B	193	ARG
1	B	214	LEU
1	B	217	LEU
1	B	244	LEU
1	B	253	ARG
1	B	270	LYS
1	B	278	VAL
1	B	279	VAL
1	B	297	ASP
1	B	317	LYS
1	B	330	ARG
1	B	366	THR
1	B	377	LEU
1	B	378	THR
1	B	418	ASP
1	B	459	LEU
1	B	475	HIS
1	B	493	SER
1	B	520	LYS

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Mol	Chain	Res	Type
1	B	538	ASN
1	B	543	THR
1	B	559	LEU
1	B	560	GLN
1	B	594	GLU
1	B	597	LEU
1	B	609	ARG
1	B	632	THR
1	B	633	SER
1	B	675	GLN
1	B	744	ASP
1	B	775	CYS
1	B	783	ASP
1	B	786	ASP
1	B	793	SER
1	B	805	SER
1	B	814	LYS
1	B	828	ARG
1	B	844	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	310	GLN
1	A	434	HIS
1	A	453	HIS
1	A	472	GLN
1	A	485	GLN
1	A	780	GLN
1	B	67	GLN
1	B	116	ASN
1	B	119	HIS
1	B	143	HIS
1	B	243	HIS
1	B	258	GLN
1	B	298	HIS
1	B	379	ASN
1	B	533	HIS
1	B	538	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.66	0	17,19,21	1.65	3 (17%)
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	1.44	4 (23%)
3	NAG	D	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	1.54	3 (17%)
3	NAG	D	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.96	5 (29%)
3	BMA	D	3	3	11,11,12	1.08	1 (9%)	15,15,17	1.65	2 (13%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	C2-C3	2.52	1.56	1.52
3	D	2	NAG	O5-C1	-2.20	1.40	1.43
3	D	1	NAG	O5-C1	-2.02	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	4.35	118.02	112.19
3	D	3	BMA	C1-C2-C3	4.19	115.75	109.64
3	D	1	NAG	O5-C1-C2	-3.98	105.13	111.29
3	D	2	NAG	C1-O5-C5	3.56	116.96	112.19
3	D	2	NAG	O4-C4-C5	3.49	117.92	109.32
3	D	2	NAG	O5-C5-C6	-3.29	101.25	107.66
3	D	1	NAG	C1-O5-C5	3.22	116.50	112.19
3	D	2	NAG	O4-C4-C3	-3.19	102.86	110.38
3	D	3	BMA	C2-C3-C4	3.12	116.35	110.86
3	D	1	NAG	O7-C7-C8	-2.54	117.53	122.05
2	C	2	NAG	O5-C1-C2	-2.44	107.51	111.29
2	C	1	NAG	O7-C7-N2	2.43	126.27	121.98
2	C	2	NAG	O7-C7-C8	-2.38	117.83	122.05
3	D	2	NAG	C4-C3-C2	2.35	114.46	111.02
2	C	1	NAG	O7-C7-C8	-2.17	118.19	122.05
2	C	2	NAG	C3-C4-C5	-2.09	106.44	110.23
2	C	2	NAG	O7-C7-N2	2.07	125.64	121.98

There are no chirality outliers.

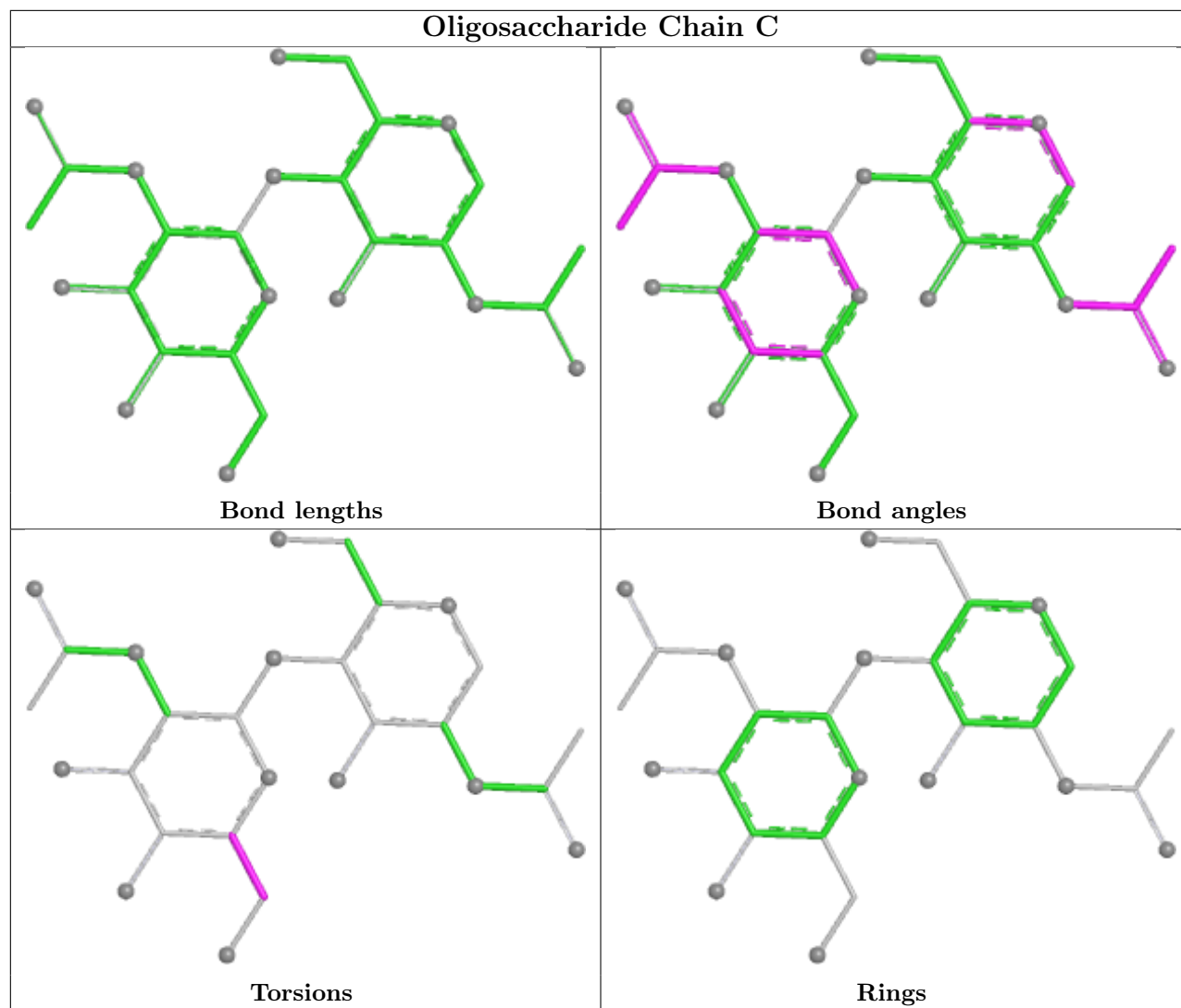
All (4) torsion outliers are listed below:

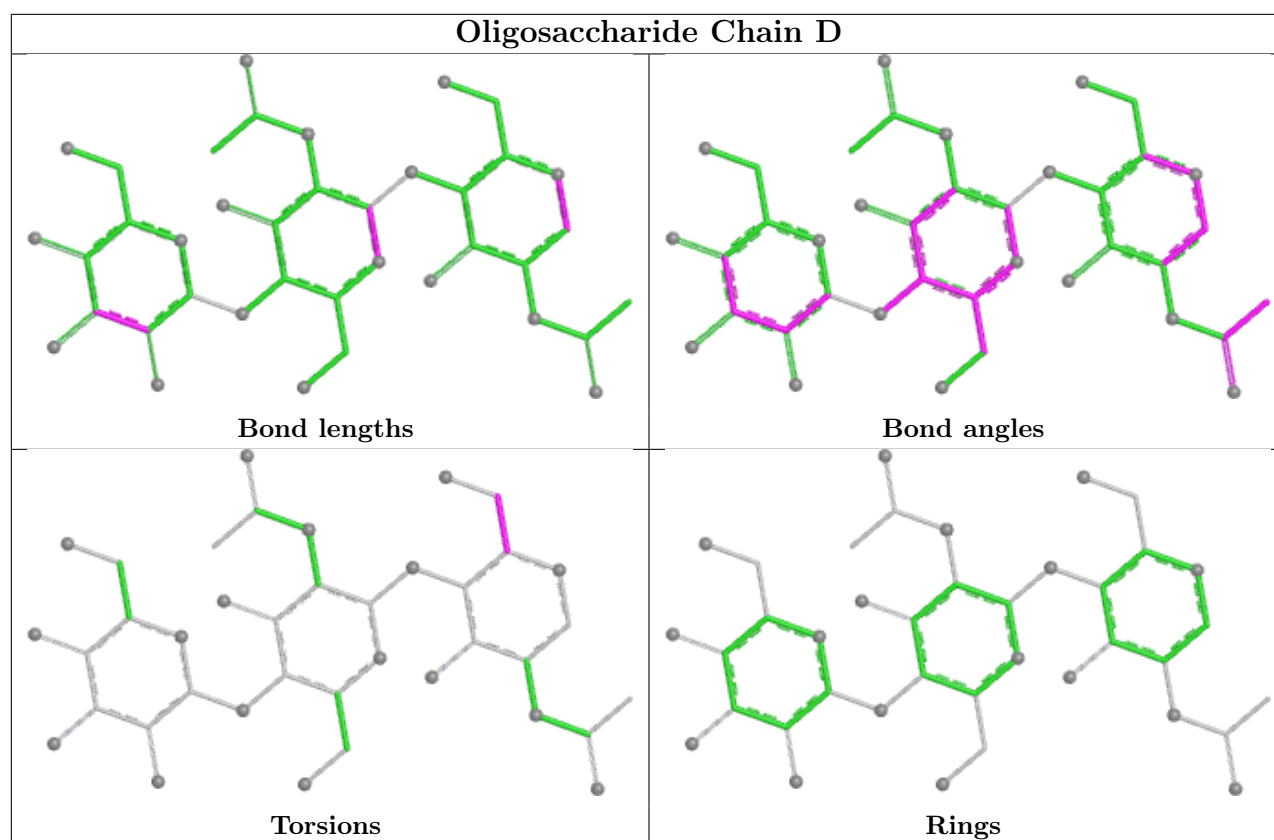
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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 [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	EDO	A	910	4	3,3,3	0.56	0	2,2,2	0.44	0
7	4O2	B	909	-	35,35,35	2.39	12 (34%)	41,52,52	2.33	10 (24%)
7	4O2	A	908	-	35,35,35	1.97	8 (22%)	41,52,52	2.25	10 (24%)
8	EDO	B	911	4	3,3,3	0.71	0	2,2,2	0.24	0
8	EDO	A	911	-	3,3,3	0.61	0	2,2,2	0.36	0
7	4O2	B	910	-	35,35,35	2.29	12 (34%)	41,52,52	2.39	11 (26%)
7	4O2	A	909	-	35,35,35	2.09	9 (25%)	41,52,52	2.25	17 (41%)

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
8	EDO	A	910	4	-	0/1/1/1	-
7	4O2	B	909	-	-	3/9/37/37	0/5/5/5
7	4O2	A	908	-	-	3/9/37/37	0/5/5/5
8	EDO	B	911	4	-	1/1/1/1	-
8	EDO	A	911	-	-	0/1/1/1	-
7	4O2	B	910	-	-	4/9/37/37	0/5/5/5
7	4O2	A	909	-	-	3/9/37/37	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	909	4O2	C10-C15	5.68	1.48	1.41
7	B	910	4O2	C4-N	-5.54	1.31	1.38
7	A	909	4O2	C5-C4	-5.42	1.45	1.52
7	B	909	4O2	C4-N	-5.35	1.31	1.38
7	A	908	4O2	C10-C15	5.20	1.47	1.41
7	B	909	4O2	C5-C4	-5.09	1.45	1.52
7	A	908	4O2	C5-C4	-5.00	1.45	1.52
7	B	909	4O2	C-N	-4.74	1.30	1.39
7	B	910	4O2	C5-C4	-4.72	1.46	1.52
7	B	910	4O2	C8-N2	-4.38	1.31	1.38
7	B	910	4O2	C-N	-4.08	1.31	1.39
7	A	908	4O2	O3-C4	4.06	1.29	1.22
7	B	909	4O2	C8-N2	-4.01	1.32	1.38
7	A	909	4O2	O3-C4	3.95	1.29	1.22
7	B	909	4O2	C15-N2	-3.77	1.32	1.39
7	A	908	4O2	O1-C3	3.76	1.34	1.22
7	A	909	4O2	O1-C3	3.65	1.34	1.22
7	B	910	4O2	C10-C15	3.63	1.45	1.41
7	B	910	4O2	C15-N2	-3.59	1.33	1.39
7	B	909	4O2	C-N1	-3.51	1.29	1.37
7	A	908	4O2	O-C	3.36	1.28	1.22
7	B	909	4O2	O2-C3	-3.22	1.20	1.30
7	A	909	4O2	O-C	3.20	1.28	1.22
7	A	908	4O2	C8-C9	3.11	1.47	1.36
7	A	909	4O2	C8-C9	3.11	1.47	1.36
7	B	910	4O2	O1-C3	3.00	1.31	1.22
7	B	909	4O2	O1-C3	2.93	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	910	4O2	O2-C3	-2.92	1.21	1.30
7	B	909	4O2	C10-C15	2.87	1.44	1.41
7	A	908	4O2	C15-N2	-2.86	1.34	1.39
7	B	909	4O2	C11-C10	-2.76	1.35	1.39
7	A	908	4O2	O2-C3	-2.70	1.21	1.30
7	B	910	4O2	C8-C9	2.64	1.45	1.36
7	B	909	4O2	C8-C9	2.64	1.45	1.36
7	B	910	4O2	C-N1	-2.44	1.32	1.37
7	B	910	4O2	O3-C4	2.34	1.26	1.22
7	A	909	4O2	C10-C9	2.33	1.48	1.44
7	A	909	4O2	C8-N2	-2.27	1.34	1.38
7	B	909	4O2	C14-C15	-2.27	1.36	1.39
7	A	909	4O2	O2-C3	-2.26	1.23	1.30
7	B	910	4O2	O-C	2.04	1.26	1.22

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	908	4O2	C7-C8-C9	-8.08	118.97	125.79
7	B	910	4O2	O3-C4-N	-7.30	115.29	124.14
7	B	910	4O2	C7-C8-C9	-6.87	120.00	125.79
7	B	909	4O2	C1-N-C4	6.64	133.59	123.28
7	B	909	4O2	C7-C8-C9	-6.61	120.21	125.79
7	A	909	4O2	C1-N-C	6.02	132.14	122.91
7	B	910	4O2	C1-N-C	5.13	130.78	122.91
7	B	909	4O2	O3-C4-N	-5.04	118.03	124.14
7	B	910	4O2	C10-C9-C8	-4.81	102.03	107.55
7	A	909	4O2	C14-C15-C10	-4.63	116.78	121.95
7	A	908	4O2	C14-C15-C10	-4.61	116.81	121.95
7	A	908	4O2	C1-N-C4	4.57	130.38	123.28
7	B	909	4O2	C10-C9-C8	-4.39	102.52	107.55
7	A	908	4O2	C1-N-C	4.36	129.59	122.91
7	A	909	4O2	C17-C16-N2	-3.88	107.15	113.46
7	B	910	4O2	C1-N-C4	3.75	129.11	123.28
7	B	909	4O2	O3-C4-C5	-3.60	118.45	125.57
7	B	909	4O2	C6-C9-C8	3.50	125.52	122.92
7	B	909	4O2	C14-C15-C10	-3.39	118.16	121.95
7	A	909	4O2	C7-C8-C9	-3.39	122.93	125.79
7	A	908	4O2	O3-C4-N	-3.36	120.06	124.14
7	A	909	4O2	O3-C4-C5	-3.23	119.19	125.57
7	A	908	4O2	C10-C9-C8	-3.19	103.89	107.55
7	A	908	4O2	O3-C4-C5	-3.12	119.41	125.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	910	4O2	C2-C1-N	-3.11	104.75	111.70
7	A	909	4O2	C6-C9-C8	-2.98	120.72	122.92
7	A	908	4O2	C6-C9-C8	2.93	125.09	122.92
7	B	909	4O2	C1-N-C	2.89	127.34	122.91
7	B	910	4O2	C14-C15-C10	-2.86	118.76	121.95
7	A	909	4O2	O3-C4-N	-2.84	120.69	124.14
7	A	909	4O2	C6-C9-C10	2.80	134.68	130.85
7	A	909	4O2	C5-C6-C9	-2.79	105.16	108.84
7	A	909	4O2	C1-N-C4	2.70	127.47	123.28
7	B	910	4O2	O2-C3-O1	-2.67	116.47	123.33
7	A	909	4O2	C10-C9-C8	-2.57	104.60	107.55
7	B	909	4O2	O2-C3-O1	-2.56	116.76	123.33
7	A	909	4O2	C15-C10-C9	-2.51	105.09	107.38
7	A	909	4O2	C16-C17-C18	2.50	125.34	120.75
7	A	909	4O2	C21-C20-C19	-2.43	119.61	122.80
7	B	910	4O2	O2-C3-C2	2.43	121.68	114.00
7	B	910	4O2	O3-C4-C5	-2.32	120.99	125.57
7	B	909	4O2	O-C-N1	-2.31	122.23	125.82
7	A	909	4O2	O2-C3-C2	2.27	121.17	114.00
7	A	908	4O2	C11-C10-C15	2.26	121.84	119.24
7	A	909	4O2	C16-N2-C15	2.08	127.98	124.79
7	B	910	4O2	C6-C9-C10	2.07	133.68	130.85
7	A	909	4O2	O-C-N1	-2.05	122.62	125.82
7	A	908	4O2	O2-C3-O1	-2.04	118.08	123.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	909	4O2	N-C1-C2-C3
7	A	909	4O2	C2-C1-N-C4
7	A	909	4O2	C2-C1-N-C
7	B	909	4O2	N-C1-C2-C3
7	B	909	4O2	C2-C1-N-C
7	B	909	4O2	C2-C1-N-C4
7	B	910	4O2	C1-C2-C3-O2
7	B	910	4O2	C1-C2-C3-O1
7	A	908	4O2	C2-C1-N-C4
7	A	908	4O2	C2-C1-N-C
7	A	908	4O2	N-C1-C2-C3
8	B	911	EDO	O1-C1-C2-O2
7	B	910	4O2	C2-C1-N-C4

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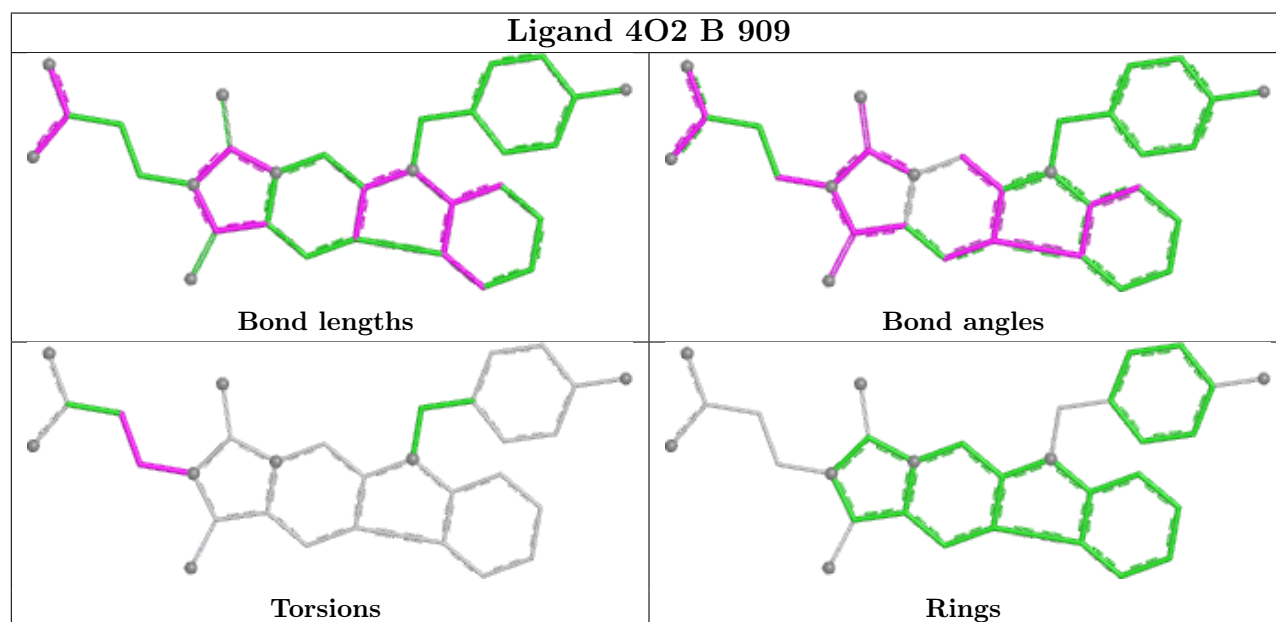
Mol	Chain	Res	Type	Atoms
7	B	910	4O2	N-C1-C2-C3

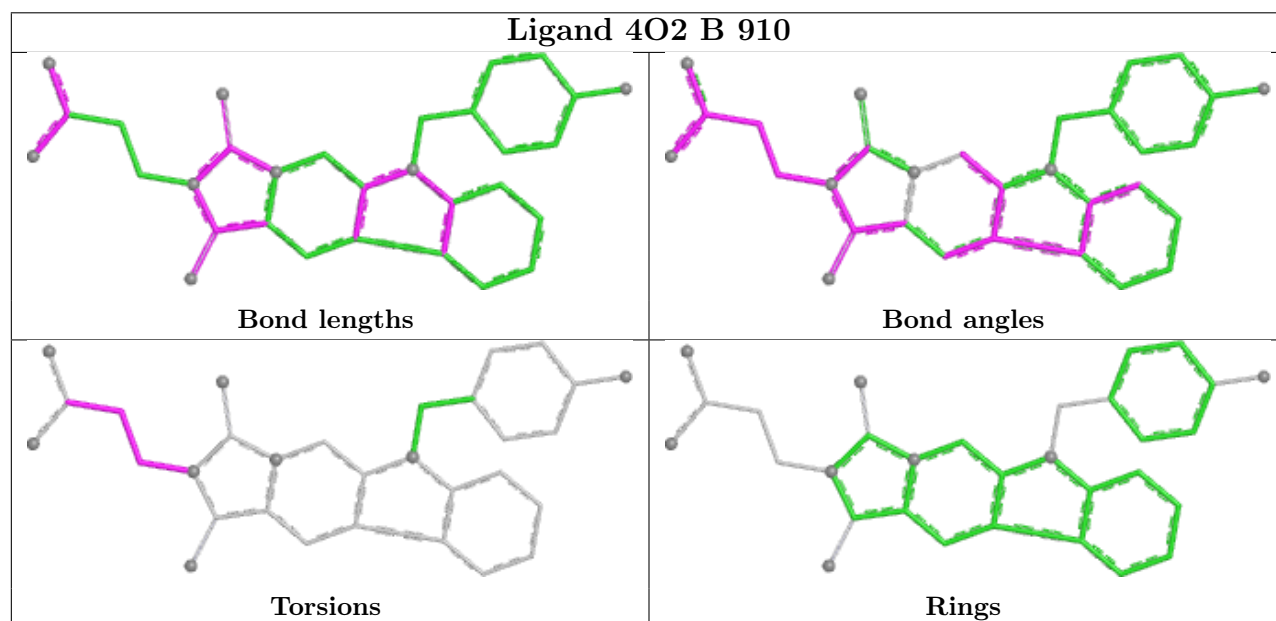
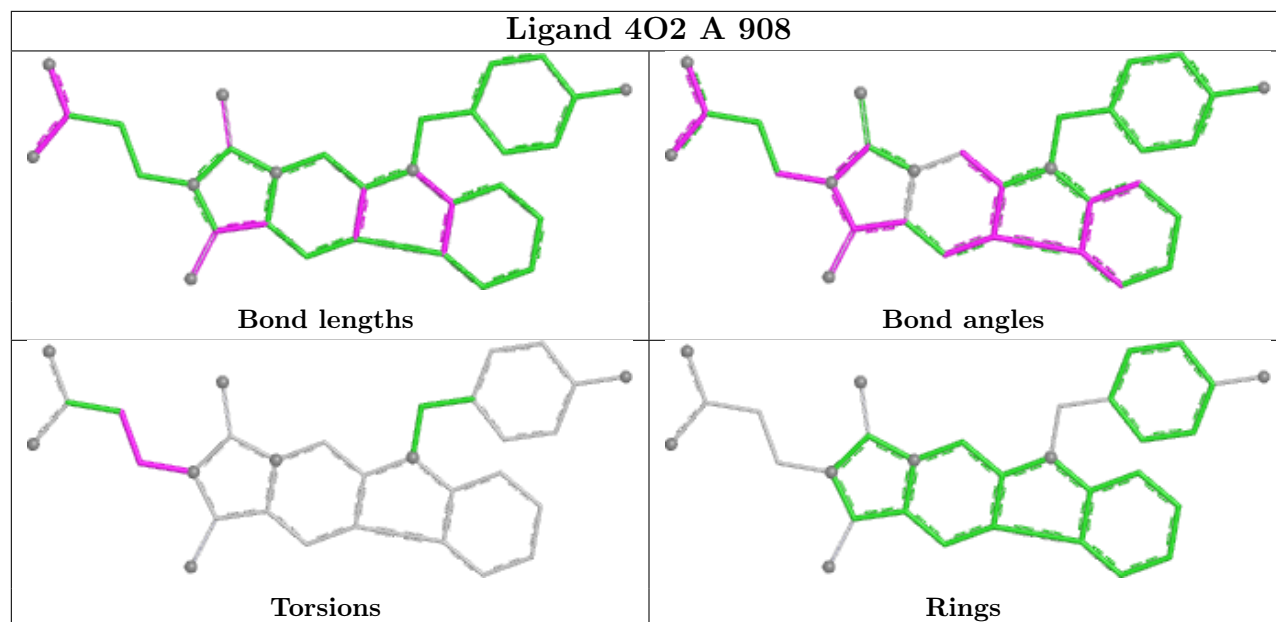
There are no ring outliers.

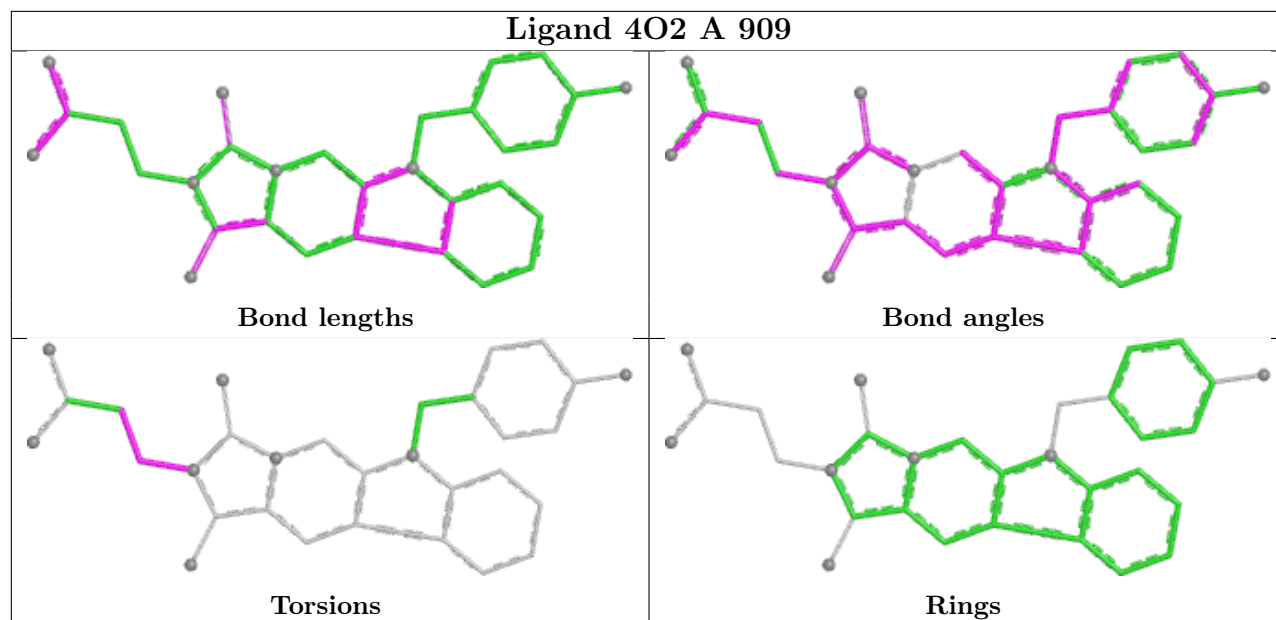
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	909	4O2	3	0
7	A	908	4O2	1	0
7	B	910	4O2	1	0
7	A	909	4O2	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	750/863 (86%)	-0.06	29 (3%)	43 35	23, 56, 104, 135	2 (0%)
1	B	764/863 (88%)	-0.07	25 (3%)	49 42	35, 57, 102, 124	0
All	All	1514/1726 (87%)	-0.07	54 (3%)	46 38	23, 57, 102, 135	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	PRO	5.9
1	B	248	GLU	5.4
1	B	861	SER	4.9
1	B	73	ASP	4.9
1	A	566	GLY	4.8
1	A	72	PRO	4.6
1	A	111	VAL	4.3
1	A	67	GLN	4.1
1	B	249	LYS	3.6
1	B	378	THR	3.5
1	B	567	CYS	3.1
1	B	126	ALA	3.1
1	B	123	ASP	2.9
1	A	118	CYS	2.7
1	A	470	PHE	2.7
1	A	84	THR	2.7
1	A	364	ASP	2.6
1	B	92	GLU	2.6
1	A	649	LEU	2.5
1	A	399	ASN	2.5
1	A	647	ASP	2.5
1	B	652	CYS	2.5
1	B	84	THR	2.5
1	B	399	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	565	LEU	2.4
1	B	239	ASP	2.4
1	A	125	LEU	2.4
1	B	231	ASN	2.4
1	A	250	PHE	2.4
1	A	651	SER	2.3
1	B	88	HIS	2.3
1	A	63	CYS	2.3
1	B	112	ARG	2.3
1	B	129	ASP	2.3
1	A	74	CYS	2.2
1	B	111	VAL	2.2
1	A	112	ARG	2.2
1	A	537	THR	2.2
1	A	652	CYS	2.2
1	B	59	CYS	2.2
1	B	321	PHE	2.1
1	B	462	TYR	2.1
1	A	252[A]	HIS	2.1
1	A	650	THR	2.1
1	A	648	HIS	2.1
1	A	458	PRO	2.1
1	A	321	PHE	2.1
1	A	368	ASP	2.1
1	B	380	VAL	2.1
1	A	130	CYS	2.0
1	B	157	CYS	2.0
1	B	245	ARG	2.0
1	A	184	LYS	2.0
1	B	465	PRO	2.0

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

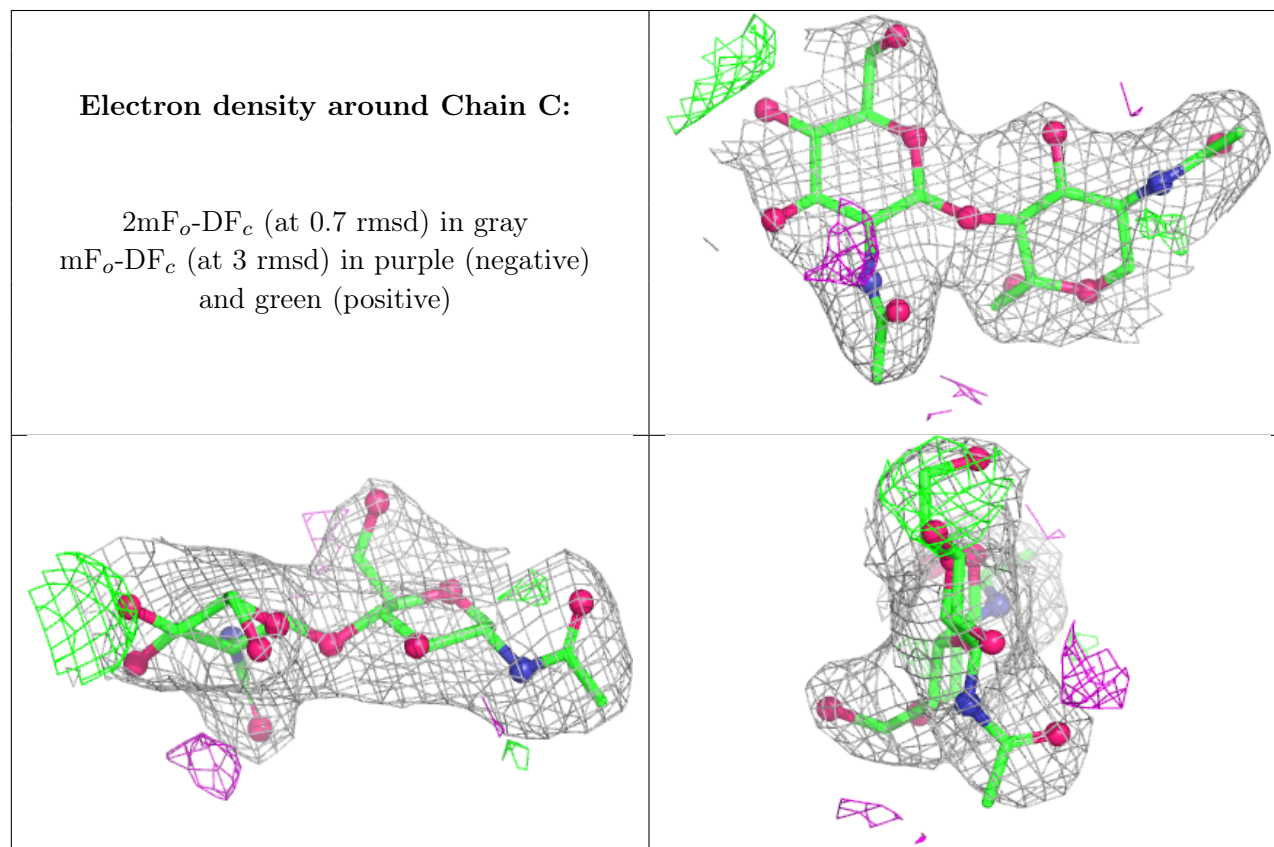
There are no non-standard protein/DNA/RNA residues in this entry.

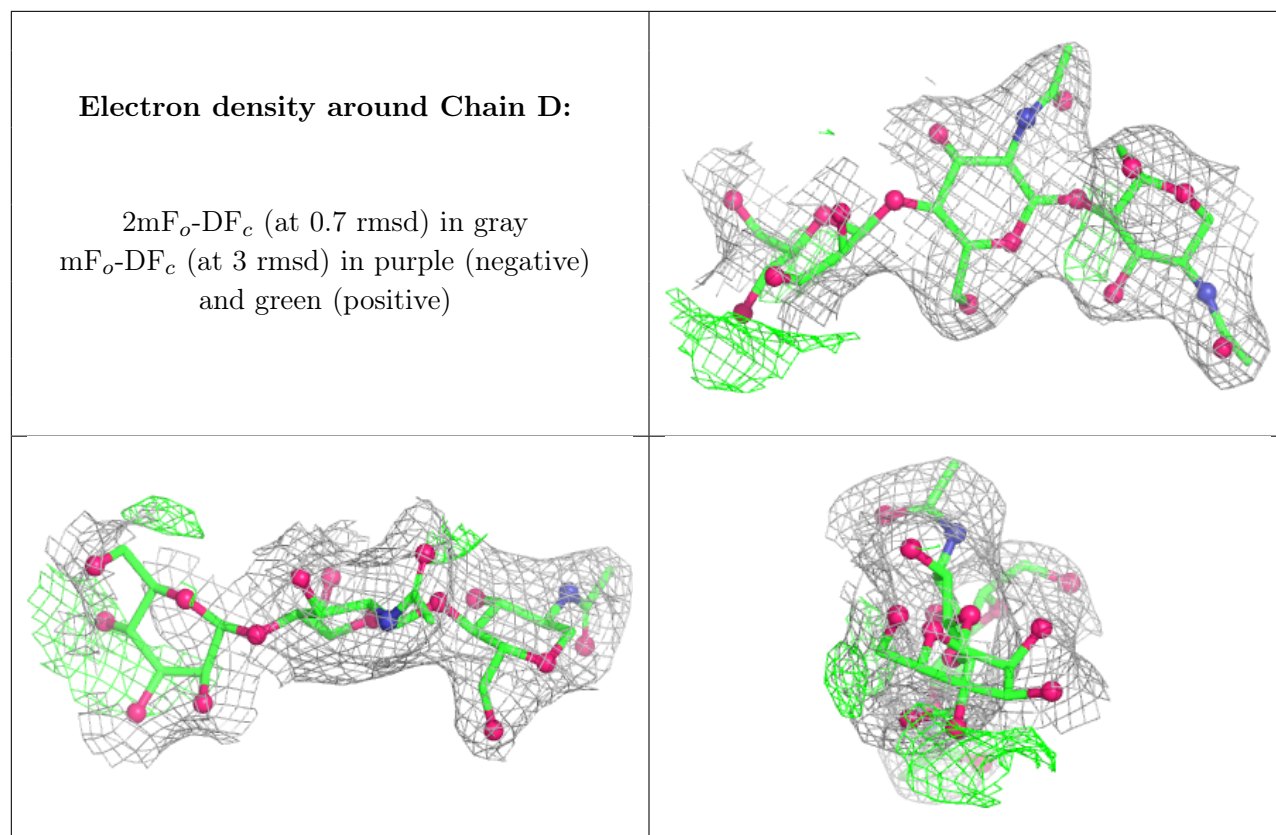
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	BMA	D	3	11/12	0.63	0.13	83,91,97,101	0
2	NAG	C	2	14/15	0.88	0.11	51,58,72,74	0
3	NAG	D	2	14/15	0.95	0.07	51,58,72,80	0
3	NAG	D	1	14/15	0.96	0.09	42,47,52,59	0
2	NAG	C	1	14/15	0.97	0.08	44,47,53,58	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($\text{\AA}^2$)	Q<0.9
6	NA	A	906	1/1	0.84	0.21	72,72,72,72	0
7	4O2	A	909	31/31	0.91	0.13	53,70,99,108	0
6	NA	B	907	1/1	0.92	0.14	56,56,56,56	0
7	4O2	B	910	31/31	0.92	0.10	50,58,87,88	0
8	EDO	A	910	4/4	0.92	0.20	48,53,55,59	0
8	EDO	B	911	4/4	0.93	0.16	46,55,61,62	0
7	4O2	B	909	31/31	0.96	0.08	42,46,69,74	0
7	4O2	A	908	31/31	0.96	0.09	37,41,54,64	0
8	EDO	A	911	4/4	0.97	0.10	44,46,48,49	0
4	ZN	B	905	1/1	0.98	0.16	93,93,93,93	0
6	NA	B	908	1/1	0.98	0.04	56,56,56,56	0
6	NA	A	907	1/1	0.98	0.09	50,50,50,50	0
5	CA	B	906	1/1	0.99	0.02	45,45,45,45	0
4	ZN	A	904	1/1	0.99	0.07	99,99,99,99	0

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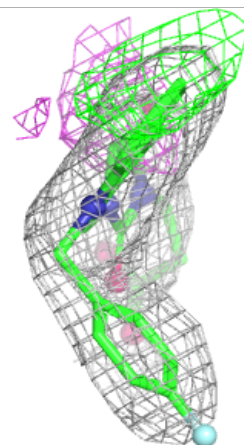
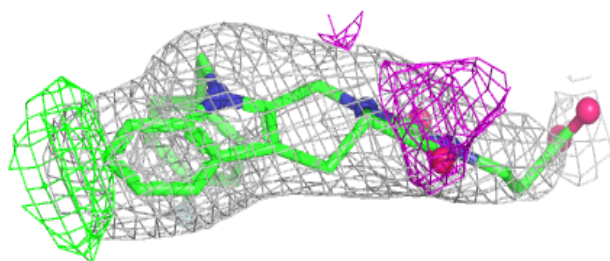
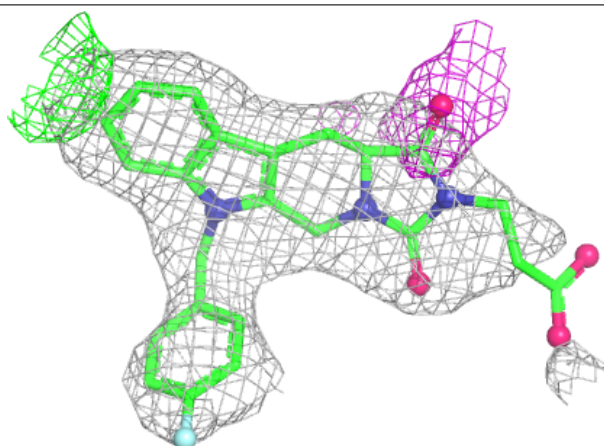
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	905	1/1	0.99	0.03	58,58,58,58	0
4	ZN	A	903	1/1	1.00	0.03	46,46,46,46	0
4	ZN	B	904	1/1	1.00	0.02	57,57,57,57	0

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.

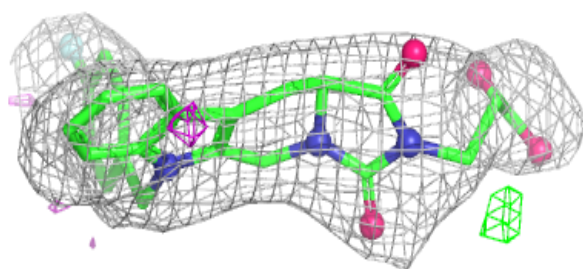
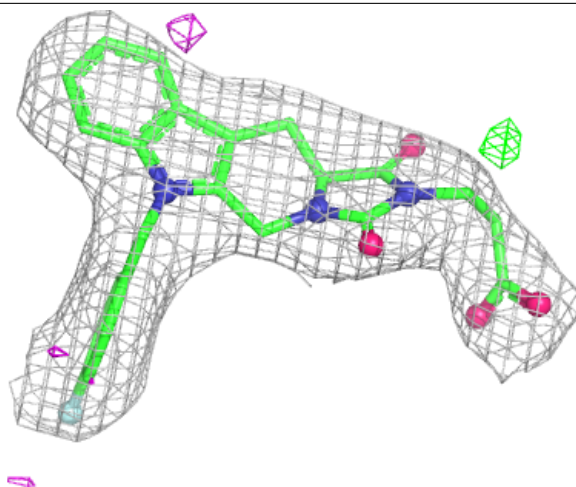
Electron density around 4O2 A 909:

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



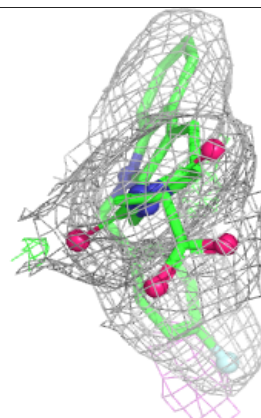
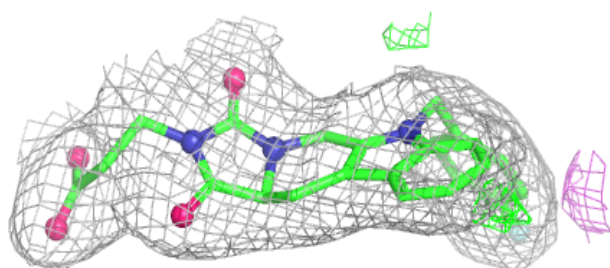
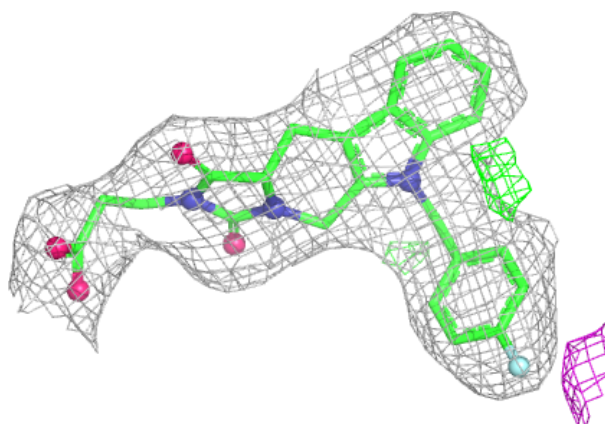
Electron density around 4O2 B 910:

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and green (positive)

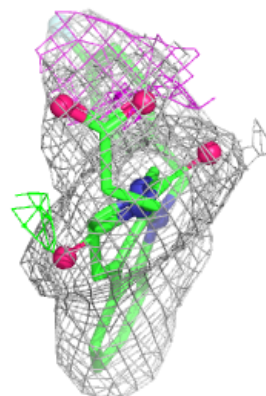
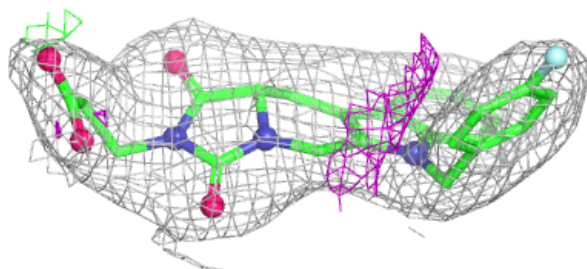
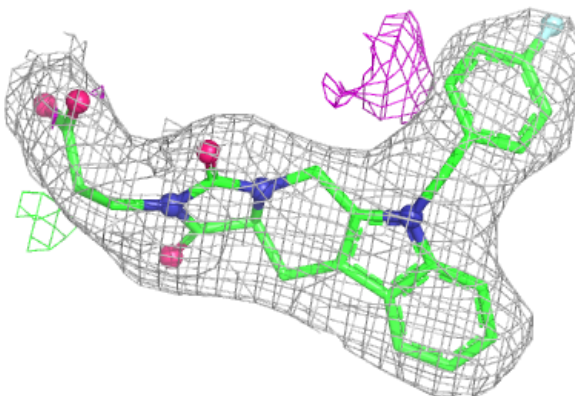


Electron density around 4O2 B 909:

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

**Electron density around 4O2 A 908:**

$2mF_o-DF_c$ (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.