



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 AM UTC

PDB ID : 5XOO / pdb_00005xoo
Title : The structure of hydra Fam20 with sugar
Authors : Zhang, H.; Xiao, J.
Deposited on : 2017-05-29
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

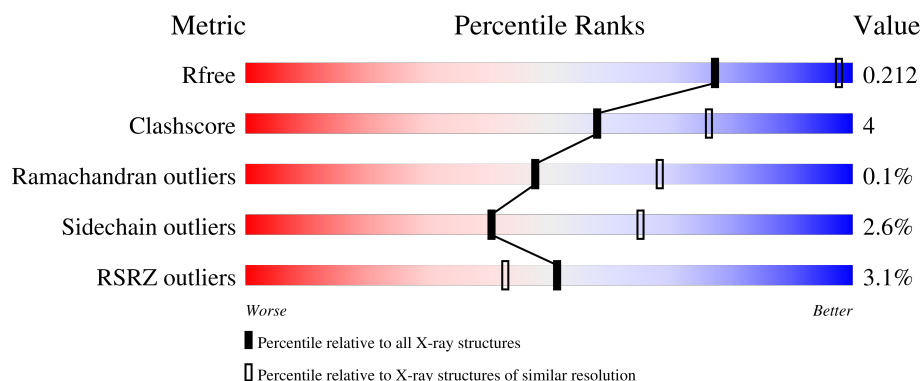
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

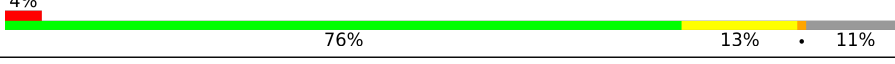
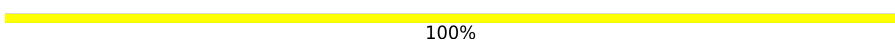
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	393	 2% 77% 11% 11%
1	B	393	 4% 76% 13% 11%
2	C	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5787 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 Glycosaminoglycan xylosylkinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2822	1812	485	511	14			
1	B	351	Total	C	N	O	S	0	0	0
			2843	1826	487	516	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP T2MHS6
B	23	GLY	-	expression tag	UNP T2MHS6

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-xylopyranose.



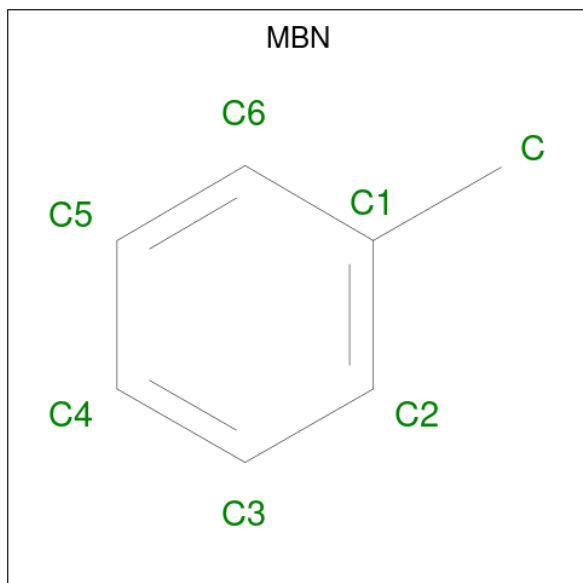
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			21	11	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



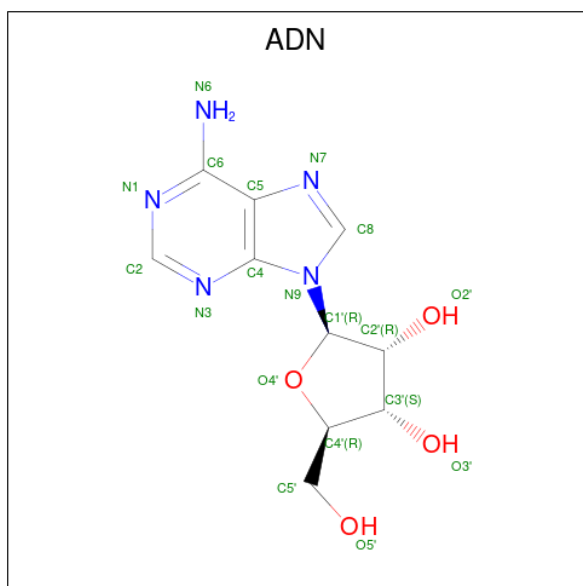
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is TOLUENE (CCD ID: MBN) (formula: C_7H_8).



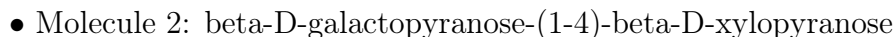
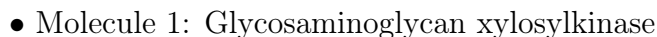
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 7 7	0	0

- Molecule 5 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 19 10 5 4	0	0
5	B	1	Total C N O 19 10 5 4	0	0

- Molecule 1: Glycosaminoglycan xylosylkinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.60Å 123.58Å 143.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.23 – 2.85 41.23 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.23-2.85) 89.5 (41.23-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.200 , 0.217 0.198 , 0.212	Depositor DCC
R_{free} test set	1609 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.4	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	0.93	EDS
Total number of atoms	5787	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, MBN, GAL, XYP, ADN

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	0.16	0/2889	0.34	0/3916
1	B	0.16	0/2911	0.35	0/3946
All	All	0.16	0/5800	0.35	0/7862

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

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	2822	0	2837	23	0
1	B	2843	0	2853	28	0
2	C	21	0	10	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	7	0	7	0	0
5	A	19	0	13	2	0
5	B	19	0	13	2	0
All	All	5787	0	5785	52	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 (52) 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:139:ARG:NH1	1:B:376:PRO:O	2.21	0.72
1:B:259:LYS:HD3	1:B:259:LYS:H	1.56	0.70
1:B:95:VAL:HG12	1:B:99:MET:HE2	1.75	0.68
1:A:86:VAL:O	1:A:165:ARG:NH1	2.29	0.65
1:B:96:LEU:HA	1:B:99:MET:HE3	1.78	0.65
1:A:294:LEU:O	1:A:389:ARG:NH1	2.29	0.65
1:A:304:GLU:OE1	5:A:506:ADN:O2'	2.13	0.64
1:B:139:ARG:NH2	1:B:229:GLU:OE2	2.32	0.62
1:A:105:THR:O	1:A:106:GLN:NE2	2.35	0.58
1:A:70:HIS:CE1	1:A:125:PRO:HD2	2.38	0.58
1:A:81:VAL:HG13	1:A:82:ARG:HG2	1.85	0.57
1:B:335:SER:HA	1:B:338:VAL:HG22	1.87	0.55
1:A:178:ARG:HD3	1:A:232:LEU:HD11	1.89	0.54
1:A:362:SER:HB2	1:A:383:LEU:HB3	1.88	0.54
1:A:111:TYR:CD2	5:A:506:ADN:H4'	2.44	0.53
1:B:81:VAL:HG13	1:B:82:ARG:HG2	1.90	0.53
1:B:385:ALA:O	1:B:389:ARG:HG3	2.08	0.53
1:B:362:SER:HB2	1:B:383:LEU:HB3	1.91	0.53
1:B:245:LEU:HD12	1:B:281:ARG:HH12	1.74	0.52
1:A:169:PHE:HB3	1:A:171:ARG:HG3	1.93	0.49
1:B:99:MET:HE1	1:B:174:PRO:HB2	1.93	0.49
1:B:169:PHE:HB3	1:B:171:ARG:HG3	1.95	0.49
5:B:503:ADN:H5'1	5:B:503:ADN:H8	1.94	0.49
1:A:171:ARG:NE	1:A:313:MET:HE2	2.29	0.48
1:B:150:GLY:O	1:B:321:LYS:HE2	2.14	0.48
1:A:329:ASP:OD1	1:A:388:ARG:NH1	2.46	0.48
1:B:159:ALA:HA	1:B:369:LEU:HD21	1.96	0.47
1:A:375:TYR:CD1	1:A:376:PRO:HA	2.50	0.46
1:B:357:ASN:HD22	1:B:364:LEU:HD11	1.81	0.46
1:B:284:ASP:O	1:B:288:THR:HG23	2.15	0.45
1:B:352:LYS:HD2	1:B:352:LYS:HA	1.66	0.45
1:A:135:LYS:HB2	1:A:154:HIS:CE1	2.52	0.44
1:A:284:ASP:OD1	1:A:344:ARG:NH2	2.51	0.44
1:B:239:LYS:HG2	1:B:240:TRP:CD1	2.53	0.44
1:B:255:LYS:HA	1:B:255:LYS:HD2	1.78	0.44
1:B:288:THR:HG22	1:B:316:HIS:NE2	2.33	0.44
1:B:178:ARG:HD3	1:B:232:LEU:HD11	1.99	0.44
1:B:86:VAL:O	1:B:165:ARG:NH1	2.50	0.44
1:A:223:ALA:HB2	1:A:228:MET:HB2	2.00	0.43
1:A:267:CYS:O	1:A:271:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:SD	1:B:234:LEU:HG	2.58	0.43
1:B:247:HIS:O	1:B:250:ARG:HG3	2.18	0.43
1:A:211:LYS:HB2	1:A:211:LYS:HE2	1.82	0.42
1:B:161:PHE:CE1	1:B:174:PRO:HA	2.55	0.42
1:B:257:MET:HE3	1:B:262:THR:HG22	2.03	0.41
1:A:368:ARG:O	1:A:371:ILE:HG12	2.20	0.41
1:B:342:ARG:HB3	1:B:411:ILE:HD13	2.03	0.41
1:B:304:GLU:OE1	5:B:503:ADN:O2'	2.21	0.41
1:A:225:ASN:HB3	1:A:226:VAL:H	1.69	0.40
1:A:119:MET:HE2	1:A:119:MET:HB2	1.90	0.40
1:A:252:THR:OG1	1:A:254:ASN:OD1	2.29	0.40
1:A:259:LYS:HD2	1:A:259:LYS:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/393 (88%)	336 (97%)	10 (3%)	1 (0%)	36	54
1	B	349/393 (89%)	339 (97%)	10 (3%)	0	100	100
All	All	696/786 (88%)	675 (97%)	20 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/354 (88%)	305 (98%)	7 (2%)	45	69
1	B	314/354 (89%)	305 (97%)	9 (3%)	37	61
All	All	626/708 (88%)	610 (97%)	16 (3%)	40	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	139	ARG
1	A	271	VAL
1	A	278	LYS
1	A	321	LYS
1	A	347	THR
1	A	360	SER
1	B	114	THR
1	B	138	SER
1	B	144	LEU
1	B	259	LYS
1	B	265	HIS
1	B	271	VAL
1	B	277	THR
1	B	352	LYS
1	B	381	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	349	ASN

5.3.3 RNA [i](#)

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	XYP	C	1	2,4	10,10,10	1.95	2 (20%)	14,14,14	1.71	1 (7%)
2	GAL	C	2	2	11,11,12	0.96	1 (9%)	15,15,17	1.16	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
2	XYP	C	1	2,4	-	-	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	XYP	O5-C1	4.46	1.50	1.43
2	C	1	XYP	O5-C5	2.70	1.48	1.43
2	C	2	GAL	O5-C1	-2.56	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	XYP	O4-C4-C3	-6.10	97.51	110.15

There are no chirality outliers.

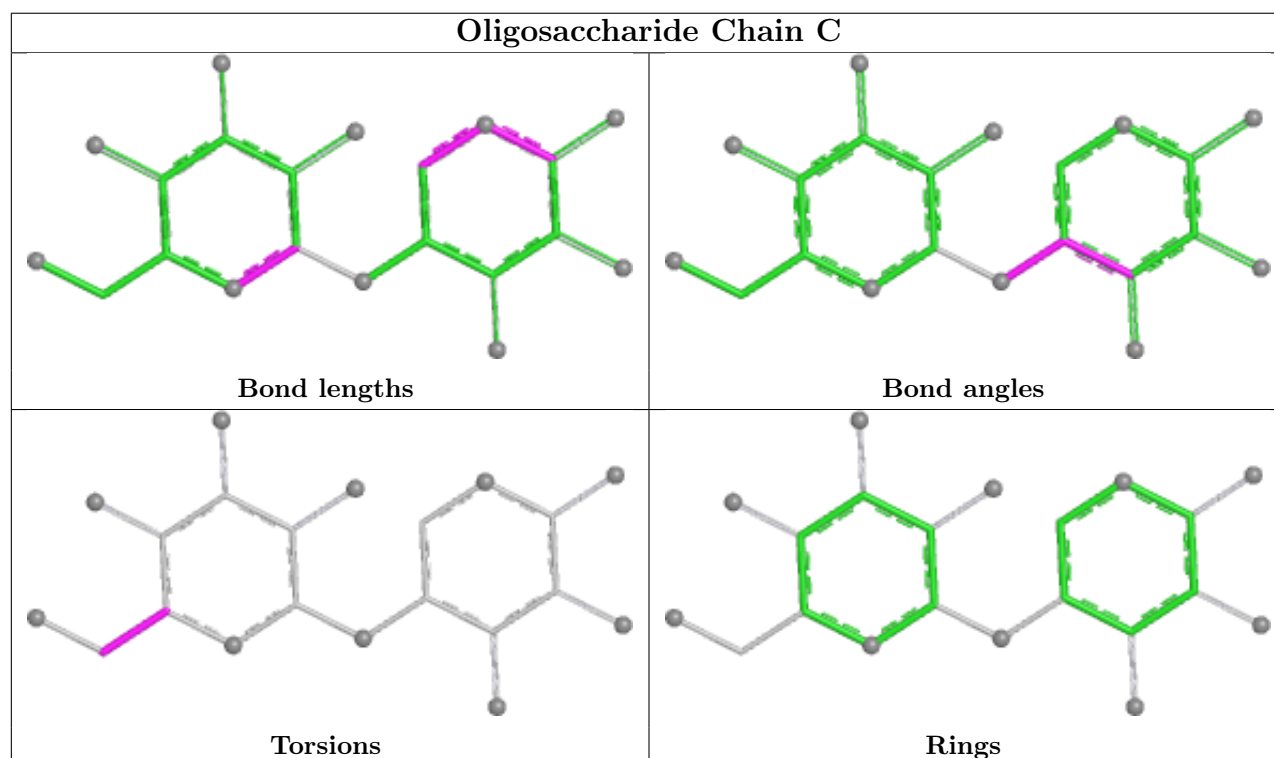
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	GAL	O5-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](#)

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	ADN	B	503	-	21,21,21	1.51	4 (19%)	31,31,31	2.38	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MBN	A	503	2	7,7,7	0.27	0	8,8,8	0.45	0
3	NAG	B	501	1	14,14,15	1.62	2 (14%)	17,19,21	2.46	1 (5%)
3	NAG	A	502	1	14,14,15	0.75	1 (7%)	17,19,21	0.61	0
3	NAG	B	502	1	14,14,15	0.42	0	17,19,21	0.39	0
5	ADN	A	506	-	21,21,21	1.50	4 (19%)	31,31,31	2.41	10 (32%)
3	NAG	A	501	1	14,14,15	1.68	2 (14%)	17,19,21	2.47	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADN	B	503	-	-	0/6/22/22	0/3/3/3
4	MBN	A	503	2	-	-	0/1/1/1
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	3/6/23/26	0/1/1/1
5	ADN	A	506	-	-	3/6/22/22	0/3/3/3
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	O5-C1	5.79	1.53	1.43
3	B	501	NAG	O5-C1	5.42	1.52	1.43
5	A	506	ADN	C6-N6	4.45	1.45	1.34
5	B	503	ADN	C6-N6	4.37	1.45	1.34
5	B	503	ADN	C5-C4	-2.89	1.33	1.39
5	A	506	ADN	C5-C4	-2.68	1.34	1.39
5	B	503	ADN	C5-N7	-2.65	1.34	1.39
5	A	506	ADN	C5-N7	-2.60	1.34	1.39
3	B	501	NAG	C1-C2	2.55	1.55	1.52
3	A	501	NAG	C1-C2	2.30	1.55	1.52
3	A	502	NAG	C1-C2	2.28	1.55	1.52
5	B	503	ADN	C8-N9	-2.09	1.34	1.37
5	A	506	ADN	C8-N9	-2.09	1.34	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-O5-C5	10.06	125.66	112.19
3	B	501	NAG	C1-O5-C5	10.02	125.62	112.19
5	A	506	ADN	N6-C6-N1	-5.86	105.32	118.38
5	B	503	ADN	N6-C6-N1	-5.71	105.65	118.38
5	B	503	ADN	N3-C2-N1	-5.71	119.94	128.58
5	A	506	ADN	N3-C2-N1	-5.42	120.38	128.58
5	A	506	ADN	C5-C4-N3	-5.41	119.26	126.72
5	B	503	ADN	C5-C4-N3	-5.24	119.50	126.72
5	A	506	ADN	C5-C6-N6	4.48	134.37	123.29
5	B	503	ADN	C5-C6-N6	4.25	133.82	123.29
5	B	503	ADN	N9-C8-N7	-3.84	108.49	113.94
5	A	506	ADN	N9-C8-N7	-3.82	108.52	113.94
5	B	503	ADN	N3-C4-N9	3.61	133.30	127.17
5	A	506	ADN	N3-C4-N9	3.53	133.17	127.17
5	B	503	ADN	C2-N3-C4	3.47	120.30	111.83
5	A	506	ADN	C2-N3-C4	3.41	120.16	111.83
5	A	506	ADN	C5-N7-C8	2.72	107.72	103.45
5	B	503	ADN	C5-N7-C8	2.49	107.37	103.45
5	A	506	ADN	C6-C5-C4	2.31	120.33	117.18
5	B	503	ADN	C4-N9-C8	2.28	108.14	105.74
5	B	503	ADN	C6-C5-C4	2.10	120.04	117.18
5	A	506	ADN	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

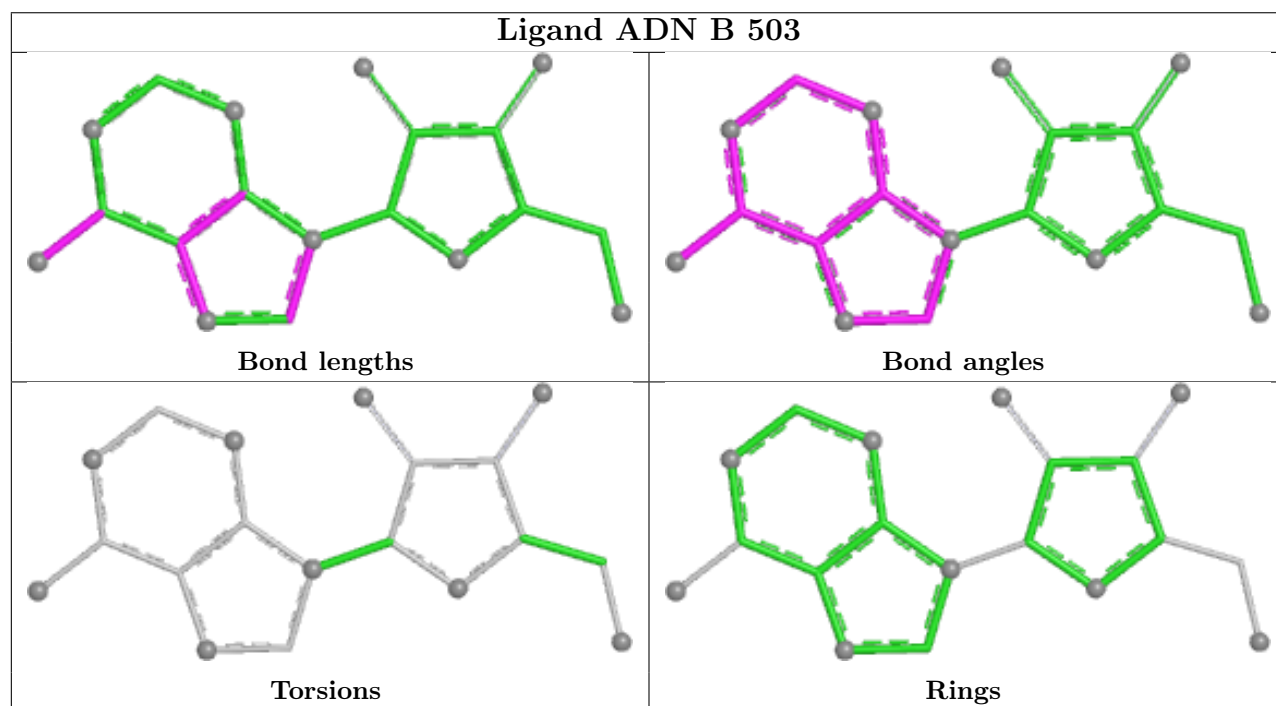
Mol	Chain	Res	Type	Atoms
5	A	506	ADN	O4'-C4'-C5'-O5'
3	B	501	NAG	O5-C5-C6-O6
5	A	506	ADN	C3'-C4'-C5'-O5'
3	B	502	NAG	O5-C5-C6-O6
3	B	501	NAG	C4-C5-C6-O6
3	B	502	NAG	C4-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
3	B	502	NAG	C3-C2-N2-C7
5	A	506	ADN	C2'-C1'-N9-C8

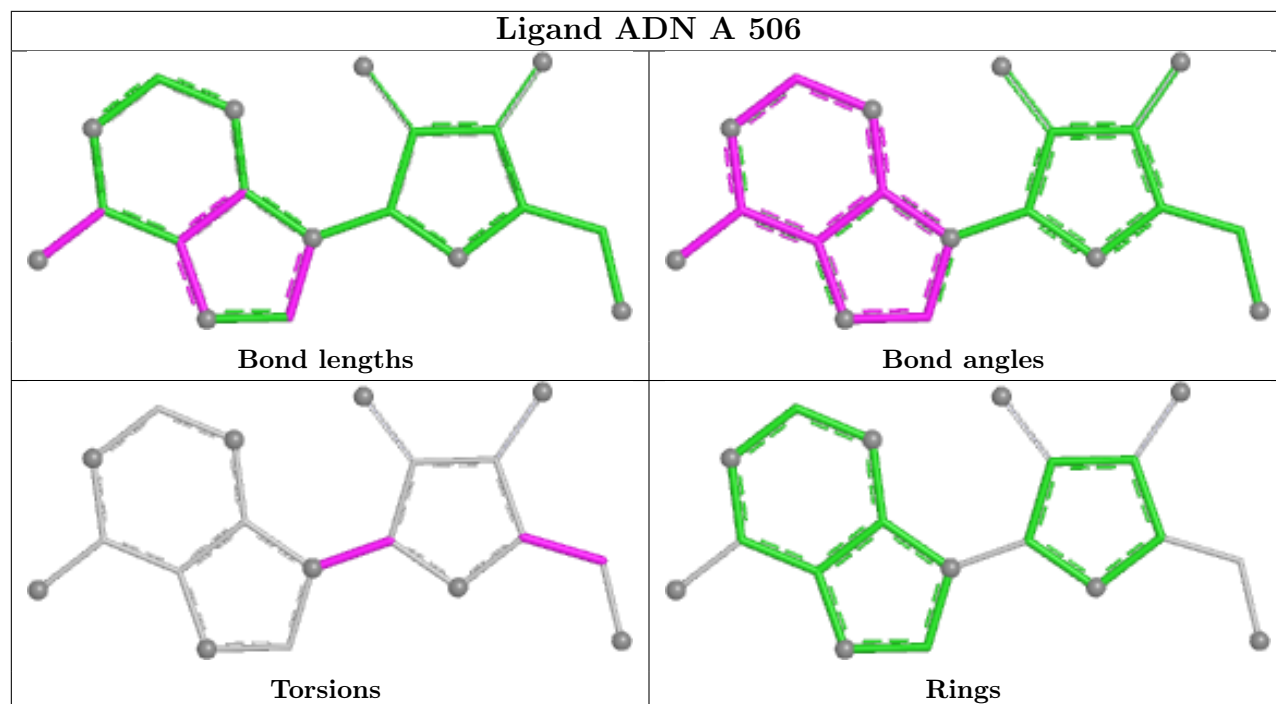
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	ADN	2	0
5	A	506	ADN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	349/393 (88%)	0.01	7 (2%) 65 57	30, 42, 76, 119	0
1	B	351/393 (89%)	0.18	15 (4%) 40 31	31, 48, 86, 117	0
All	All	700/786 (89%)	0.09	22 (3%) 51 43	30, 44, 81, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	TYR	6.0
1	B	110	GLY	5.1
1	B	111	TYR	4.4
1	B	278	LYS	3.5
1	A	110	GLY	3.2
1	B	66	TYR	3.0
1	B	145	GLY	2.9
1	B	255	LYS	2.8
1	B	352	LYS	2.7
1	A	352	LYS	2.6
1	B	259	LYS	2.6
1	B	404	LYS	2.5
1	B	113	GLY	2.4
1	B	402	LYS	2.4
1	B	403	GLU	2.4
1	B	112	LYS	2.3
1	B	149	GLU	2.3
1	B	274	GLU	2.3
1	A	380	SER	2.3
1	A	272	ILE	2.3
1	A	112	LYS	2.2
1	A	330	GLU	2.0

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

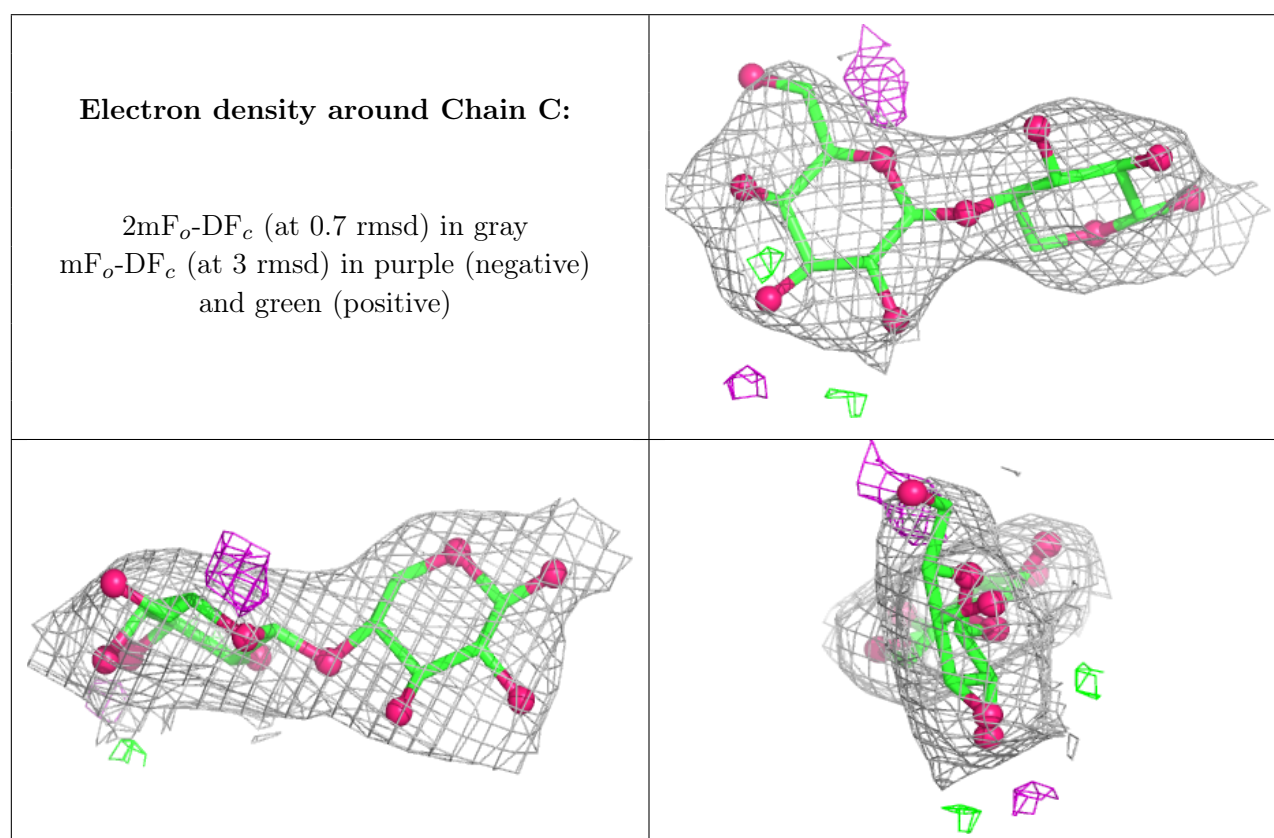
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	GAL	C	2	11/12	0.92	0.10	36,45,63,63	0
2	XYP	C	1	10/10	0.94	0.08	46,49,57,61	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.



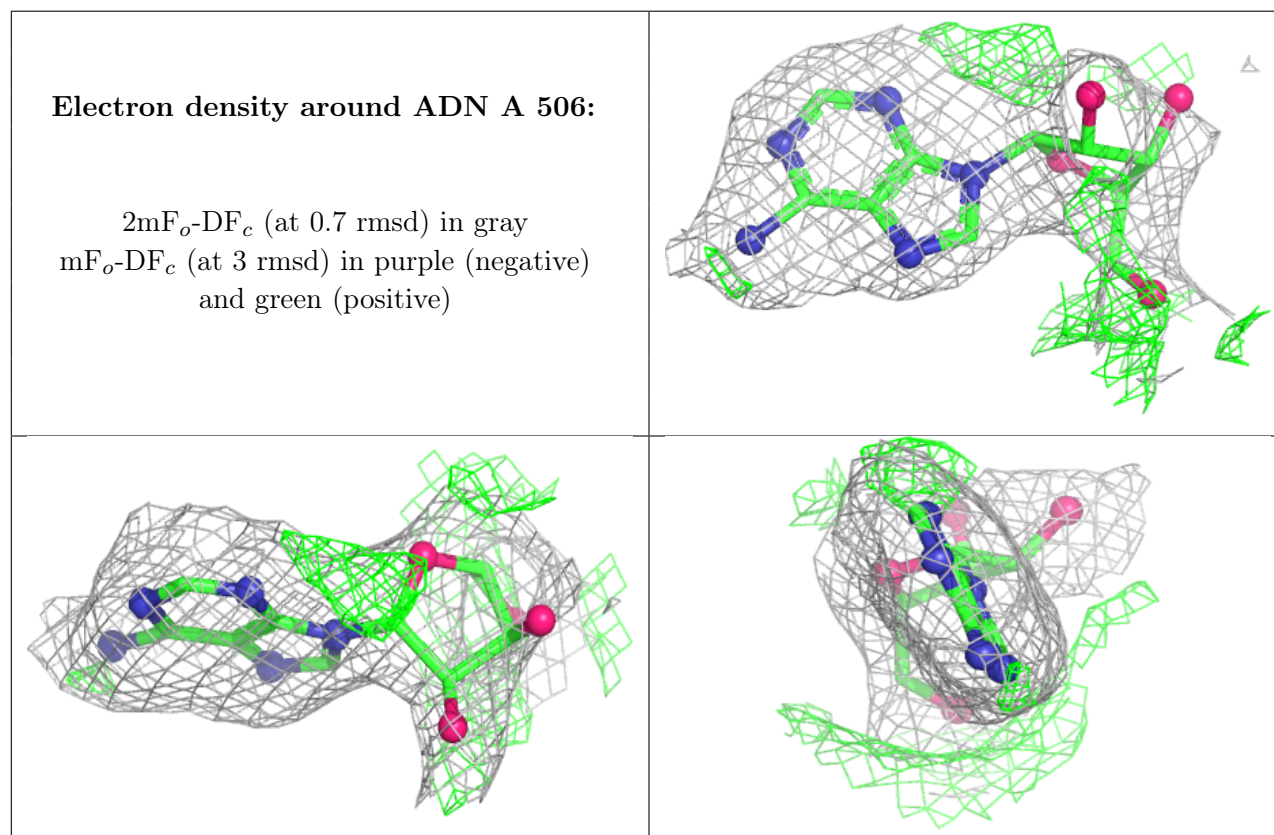
6.4 Ligands ⓘ

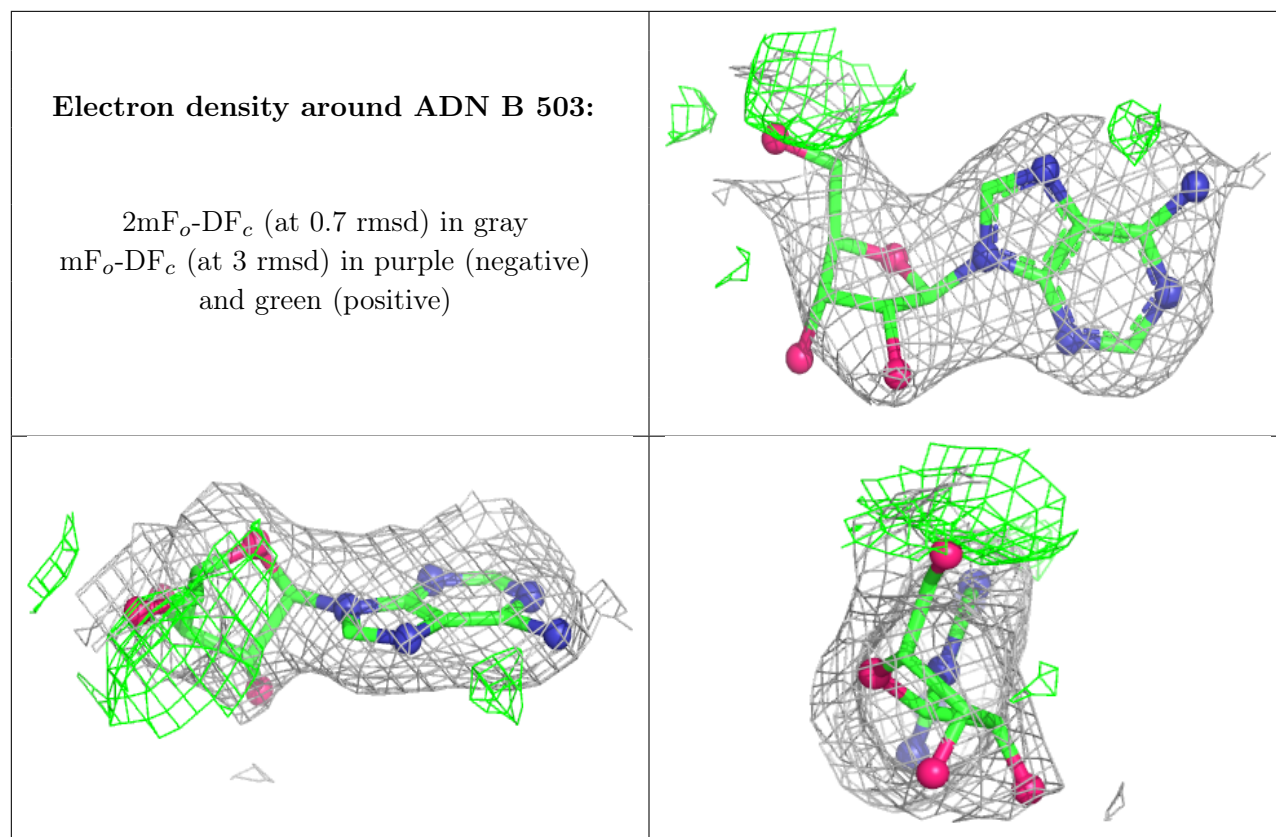
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	NAG	B	501	14/15	0.44	0.23	85,97,107,109	0
3	NAG	A	501	14/15	0.56	0.22	66,85,95,97	0
3	NAG	A	502	14/15	0.61	0.20	81,93,99,104	0
3	NAG	B	502	14/15	0.63	0.21	100,109,118,118	0
5	ADN	A	506	19/19	0.77	0.18	41,75,90,100	0
5	ADN	B	503	19/19	0.82	0.15	42,62,106,123	0
4	MBN	A	503	7/7	0.95	0.15	66,67,68,68	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.