



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 08:16 AM EDT

PDB ID : 5SVL  
Title : Crystal structure of the ATP-gated human P2X3 ion channel in the ATP-bound, closed (desensitized) state  
Authors : Mansoor, S.E.; Lu, W.; Oosterheert, W.; Shekhar, M.; Tajkhorshid, E.; Gouaux, E.  
Deposited on : 2016-08-06  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

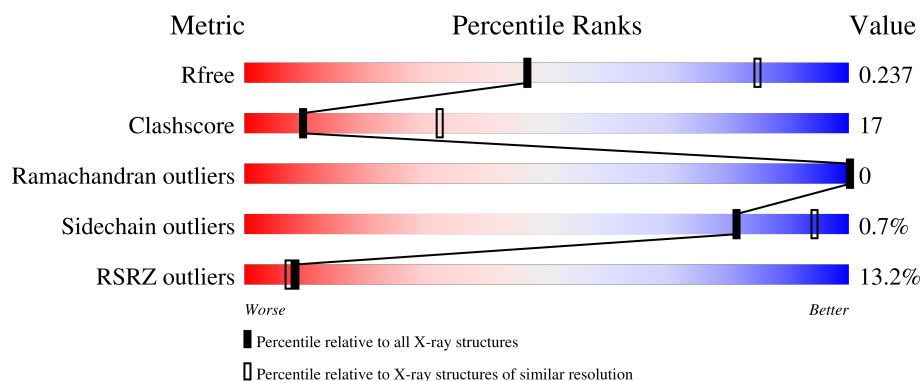
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	363	
1	B	363	
2	C	2	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5446 atoms, of which 130 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 P2X purinoceptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2565	1650	426	471	18			
1	B	318	Total	C	N	O	S	0	0	0
			2443	1574	399	452	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P56373
A	3	SER	-	expression tag	UNP P56373
A	4	ARG	-	expression tag	UNP P56373
A	5	ALA	-	expression tag	UNP P56373
B	2	GLY	-	expression tag	UNP P56373
B	3	SER	-	expression tag	UNP P56373
B	4	ARG	-	expression tag	UNP P56373
B	5	ALA	-	expression tag	UNP P56373

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



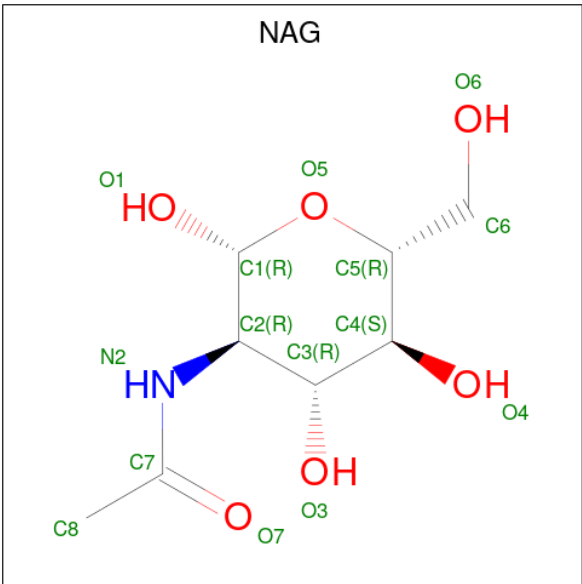
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
3	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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



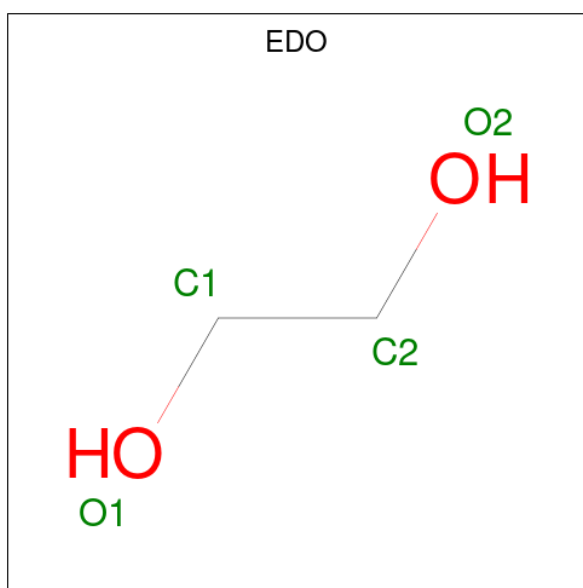
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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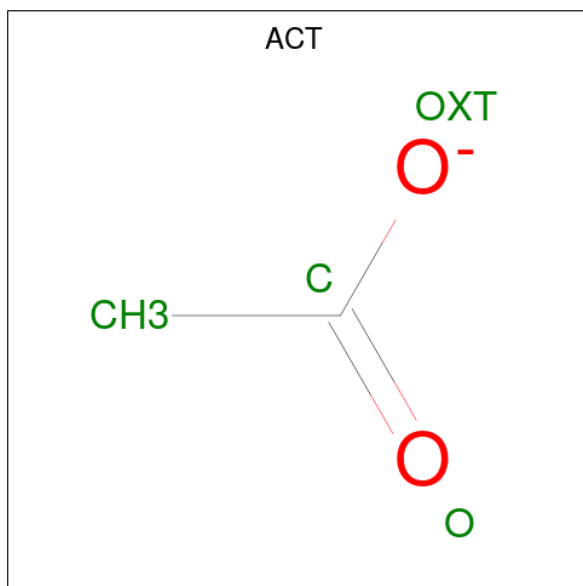
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	B	1	Total 28	C 8	H 14	N 1	O 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Na	0	0
			2	2		
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



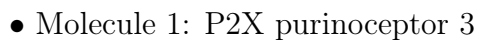
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	48	Total	O	0	0
			48	48		
9	B	44	Total	O	0	0
			44	44		



- Molecule 1: P2X purinoceptor 3





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 

  
GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.14Å 172.14Å 172.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.98 – 2.90 76.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.5 (76.98-2.90) 97.7 (76.98-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX dev_1634	Depositor
R, $R_{free}$	0.205 , 0.240 0.213 , 0.237	Depositor DCC
$R_{free}$ test set	1849 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TRS, NAG, ACT, GLC, NA, ATP, 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	0.34	0/2621	0.59	1/3558 (0.0%)
1	B	0.34	0/2497	0.58	0/3392
All	All	0.34	0/5118	0.58	1/6950 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2565	0	2526	89	1
1	B	2443	0	2387	88	1
2	C	23	22	21	0	0
3	A	31	12	12	2	0
3	B	31	12	12	2	0
4	A	42	42	39	2	0
4	B	42	42	39	2	0
5	A	16	0	24	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	8	0	12	2	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	A	8	0	12	0	0
9	A	48	0	0	4	0
9	B	44	0	0	3	0
All	All	5316	130	5093	179	1

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 17.

All (179) 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:115:ARG:HA	1:B:146:THR:HG22	1.45	0.97
1:A:31:GLN:HG2	1:A:336:THR:HG22	1.47	0.96
1:B:27:ASN:HB2	1:B:343:LEU:CD1	1.97	0.94
1:B:31:GLN:HG2	1:B:336:THR:HG22	1.49	0.94
1:A:319:ILE:HB	1:A:320:PRO:HD3	1.55	0.87
1:A:279:ASN:H	5:A:409:EDO:H22	1.38	0.84
1:B:319:ILE:HB	1:B:320:PRO:HD3	1.61	0.83
1:A:75:MET:HG3	1:A:165:MET:HE3	1.64	0.80
1:B:156:GLU:OE2	1:B:281:ARG:NH1	2.16	0.80
1:B:180:ARG:NH2	1:B:185:ASN:HA	1.97	0.79
1:A:184:PHE:HD2	1:A:249:LEU:HD12	1.51	0.76
1:A:184:PHE:CD2	1:A:249:LEU:HD12	2.23	0.73
1:A:51:VAL:HG13	1:A:320:PRO:HG2	1.69	0.73
1:A:115:ARG:HA	1:A:146:THR:HG22	1.71	0.73
1:B:212:PHE:HZ	1:B:257:ILE:HD12	1.54	0.73
1:B:212:PHE:HE1	1:B:257:ILE:HB	1.56	0.70
1:B:177:ASN:HB3	1:B:190:ASN:HB2	1.74	0.70
1:B:190:ASN:OD1	1:B:260:TYR:OH	2.10	0.69
1:A:95:LYS:HB3	1:A:301:PHE:HB2	1.73	0.69
1:B:339:CYS:O	1:B:343:LEU:HG	1.93	0.68
1:B:184:PHE:HD2	1:B:249:LEU:HD12	1.60	0.67
1:A:156:GLU:OE2	1:A:281:ARG:NH1	2.28	0.67
1:A:175:ILE:O	1:A:190:ASN:ND2	2.26	0.65
1:A:142:SER:O	5:A:408:EDO:H22	1.97	0.64
1:B:95:LYS:HB3	1:B:301:PHE:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:MET:HB2	1:A:165:MET:CE	2.27	0.64
1:A:206:HIS:HB3	1:A:209:LYS:HB2	1.80	0.63
1:B:114:TYR:HH	1:B:129:GLY:N	1.97	0.63
1:A:271:LYS:HE3	9:A:525:HOH:O	1.98	0.63
4:A:402:NAG:H62	1:B:273:SER:HB2	1.81	0.63
1:A:31:GLN:O	1:A:35:ILE:HG12	1.99	0.62
1:B:27:ASN:HB2	1:B:343:LEU:HD12	1.80	0.62
1:A:75:MET:HB2	1:A:165:MET:HE1	1.81	0.62
1:B:109:GLU:HG2	1:B:114:TYR:CD1	2.35	0.62
1:A:281:ARG:NH2	3:A:401:ATP:O3G	2.33	0.62
1:B:192:LEU:HD11	1:B:212:PHE:CD1	2.35	0.61
1:B:330:THR:O	1:B:334:VAL:HG23	2.00	0.61
1:A:51:VAL:CG1	1:A:320:PRO:HG2	2.30	0.61
1:A:109:GLU:HG2	1:A:114:TYR:CG	2.35	0.61
1:A:304:ARG:NH2	9:A:502:HOH:O	2.33	0.61
1:A:188:LYS:HE3	1:A:253:TRP:CH2	2.36	0.60
1:B:27:ASN:HB2	1:B:343:LEU:HD13	1.83	0.60
1:B:212:PHE:CE1	1:B:257:ILE:HB	2.37	0.60
1:B:279:ASN:H	5:B:406:EDO:H11	1.67	0.60
1:A:232:LEU:HD23	1:A:303:ILE:HD13	1.82	0.60
1:A:275:SER:HB2	3:A:401:ATP:H5'1	1.84	0.60
4:B:403:NAG:O7	4:B:403:NAG:O3	2.16	0.60
1:A:330:THR:O	1:A:334:VAL:HG23	2.02	0.60
1:A:278:TYR:HA	5:A:409:EDO:H21	1.84	0.59
1:B:328:ALA:O	1:B:332:VAL:HG22	2.02	0.59
1:B:327:ALA:O	1:B:330:THR:HG22	2.04	0.58
1:B:184:PHE:CD2	1:B:249:LEU:HD12	2.38	0.58
1:B:212:PHE:CZ	1:B:257:ILE:HD12	2.39	0.57
1:A:252:ALA:HB3	1:A:255:GLN:HG2	1.86	0.57
1:B:180:ARG:NH1	1:B:187:GLU:HG3	2.19	0.57
1:B:180:ARG:HH22	1:B:185:ASN:HA	1.69	0.57
1:B:164:ILE:HD11	1:B:166:MET:SD	2.44	0.57
1:A:139:ASN:ND2	5:A:408:EDO:H21	2.20	0.57
1:A:338:LEU:O	1:A:342:ILE:HG13	2.05	0.57
1:B:175:ILE:O	1:B:190:ASN:ND2	2.37	0.56
1:B:204:ARG:NH1	9:B:502:HOH:O	2.34	0.56
1:B:217:ARG:HD3	1:B:220:ASP:OD1	2.05	0.56
1:B:242:LYS:HB2	1:B:261:SER:HB3	1.87	0.55
1:A:339:CYS:O	1:A:343:LEU:HG	2.05	0.55
1:A:327:ALA:O	1:A:330:THR:HG22	2.07	0.54
1:A:69:LEU:N	1:A:167:GLU:OE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:HB2	1:A:157:VAL:HG12	1.89	0.54
1:B:75:MET:HB2	1:B:165:MET:HE1	1.90	0.54
1:B:31:GLN:HG2	1:B:336:THR:CG2	2.33	0.54
1:A:319:ILE:O	1:A:323:ILE:HG12	2.08	0.53
1:B:69:LEU:N	1:B:167:GLU:OE2	2.30	0.53
1:A:34:ILE:HD13	1:A:335:GLY:HA3	1.91	0.53
1:B:144:LEU:HD12	1:B:145:ARG:N	2.23	0.53
1:A:139:ASN:HA	1:A:145:ARG:HG3	1.91	0.53
1:A:157:VAL:HG22	9:A:529:HOH:O	2.08	0.53
1:A:185:ASN:O	1:A:185:ASN:ND2	2.42	0.53
1:A:169:GLU:HG2	1:A:217:ARG:NH2	2.25	0.52
1:B:75:MET:HG3	1:B:165:MET:HE3	1.92	0.52
1:B:281:ARG:NH2	3:B:401:ATP:O3G	2.43	0.52
1:A:328:ALA:O	1:A:332:VAL:HG22	2.08	0.52
1:A:31:GLN:HG2	1:A:336:THR:CG2	2.31	0.51
1:A:195:LEU:HD12	1:A:199:ASP:CB	2.40	0.51
1:B:138:VAL:HG12	1:B:139:ASN:N	2.25	0.51
1:B:29:VAL:O	1:B:33:LEU:HD13	2.10	0.51
1:B:338:LEU:O	1:B:342:ILE:HG13	2.11	0.51
1:A:138:VAL:HG12	1:A:139:ASN:N	2.25	0.51
1:B:329:PHE:HA	1:B:332:VAL:CG2	2.41	0.50
1:B:134:THR:OG1	1:B:148:GLU:HB3	2.12	0.50
1:B:180:ARG:HH11	1:B:187:GLU:CG	2.24	0.50
1:A:38:PHE:CE1	1:A:331:SER:HB3	2.47	0.50
1:B:206:HIS:CG	1:B:207:PRO:HD2	2.47	0.50
1:B:26:ILE:HD12	1:B:26:ILE:C	2.33	0.50
1:B:329:PHE:HA	1:B:332:VAL:HG22	1.92	0.50
1:A:217:ARG:HD3	1:A:220:ASP:OD1	2.13	0.49
1:A:75:MET:CG	1:A:165:MET:HE3	2.39	0.49
1:A:176:LYS:HA	1:A:191:LEU:HD11	1.95	0.49
1:B:50:GLN:HG3	1:B:315:LYS:C	2.33	0.49
1:A:26:ILE:C	1:A:26:ILE:HD12	2.34	0.48
1:B:319:ILE:O	1:B:323:ILE:HG12	2.14	0.48
1:B:83:PRO:HB2	1:B:85:GLN:OE1	2.13	0.48
1:B:107:CYS:HB2	1:B:108:PRO:HD2	1.94	0.48
1:B:36:SER:O	1:B:40:GLY:N	2.46	0.48
1:B:39:VAL:O	1:B:44:LEU:HG	2.14	0.48
1:B:181:PHE:CZ	1:B:313:ALA:HB2	2.49	0.47
1:A:139:ASN:OD1	1:A:145:ARG:HD2	2.14	0.47
1:B:144:LEU:HD12	1:B:145:ARG:H	1.80	0.47
1:B:275:SER:HB2	3:B:401:ATP:H5'1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HG23	1:B:148:GLU:HB2	1.97	0.47
1:B:180:ARG:HH11	1:B:187:GLU:HG3	1.79	0.47
1:B:245:TRP:CH2	1:B:258:PRO:HD3	2.49	0.47
1:A:25:ILE:O	1:A:29:VAL:HG23	2.14	0.47
1:B:89:VAL:HA	1:B:305:PHE:O	2.15	0.47
1:B:304:ARG:NH2	9:B:501:HOH:O	2.20	0.47
1:A:127:LEU:HB3	1:A:128:PRO:HD2	1.98	0.46
1:A:184:PHE:HD2	1:A:249:LEU:CD1	2.25	0.46
1:A:195:LEU:HD12	1:A:199:ASP:HB2	1.97	0.46
1:A:212:PHE:HZ	1:A:257:ILE:HG22	1.80	0.46
1:B:177:ASN:H	1:B:190:ASN:HB3	1.80	0.46
1:A:26:ILE:HD12	1:A:27:ASN:N	2.30	0.46
1:A:39:VAL:O	1:A:44:LEU:HG	2.16	0.46
1:A:109:GLU:HG2	1:A:114:TYR:CD1	2.50	0.46
1:A:337:VAL:O	1:A:341:ILE:HG12	2.15	0.46
1:B:31:GLN:O	1:B:35:ILE:HG12	2.16	0.46
1:B:38:PHE:CZ	1:B:331:SER:HB3	2.50	0.46
1:A:181:PHE:CE2	1:A:313:ALA:HB2	2.50	0.46
1:A:75:MET:HB2	1:A:165:MET:HE3	1.99	0.45
1:B:117:VAL:HG12	1:B:121:GLN:OE1	2.16	0.45
1:A:188:LYS:HG3	1:A:253:TRP:CZ2	2.51	0.45
1:B:134:THR:HG1	1:B:148:GLU:HB3	1.81	0.45
1:A:176:LYS:HA	1:A:191:LEU:CD1	2.46	0.45
1:A:278:TYR:HA	5:A:409:EDO:C2	2.46	0.45
1:A:144:LEU:HD12	1:A:145:ARG:N	2.32	0.45
1:A:179:ILE:HG21	1:A:245:TRP:CD1	2.52	0.45
1:B:223:LYS:HE3	9:B:509:HOH:O	2.16	0.45
1:A:30:VAL:O	1:A:34:ILE:HG13	2.16	0.45
1:B:49:TYR:HB2	1:B:321:THR:OG1	2.17	0.45
4:A:402:NAG:C6	1:B:273:SER:HB2	2.47	0.44
1:B:278:TYR:HA	5:B:406:EDO:H11	1.99	0.44
1:B:102:GLN:HA	1:B:153:CYS:O	2.17	0.44
1:B:109:GLU:HG2	1:B:114:TYR:CG	2.52	0.44
1:A:62:THR:HA	1:A:174:PHE:O	2.18	0.43
1:B:185:ASN:O	1:B:185:ASN:ND2	2.51	0.43
1:A:287:LYS:NZ	9:A:505:HOH:O	2.51	0.43
1:B:46:GLU:O	1:B:52:ARG:NH1	2.51	0.43
1:A:110:SER:CB	1:A:157:VAL:HG12	2.48	0.43
1:A:212:PHE:CZ	1:A:257:ILE:HG22	2.53	0.43
1:B:116:CYS:N	1:B:146:THR:HA	2.33	0.43
1:A:319:ILE:HB	1:A:320:PRO:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD23	1:A:184:PHE:CE1	2.54	0.43
1:B:110:SER:OG	1:B:157:VAL:HG22	2.19	0.43
1:A:157:VAL:O	1:A:157:VAL:HG23	2.19	0.43
1:B:75:MET:HB2	1:B:165:MET:CE	2.49	0.43
1:A:47:LYS:HA	1:A:49:TYR:CE1	2.54	0.43
1:A:210:ASP:N	1:A:211:PRO:HD3	2.33	0.43
1:A:43:PHE:CD2	1:A:44:LEU:HD23	2.54	0.43
1:B:30:VAL:O	1:B:34:ILE:HG12	2.19	0.43
1:A:218:VAL:O	1:A:222:VAL:HG23	2.18	0.42
1:B:50:GLN:HG3	1:B:315:LYS:O	2.18	0.42
1:A:43:PHE:HD2	1:A:44:LEU:CD2	2.32	0.42
1:A:139:ASN:HD21	5:A:408:EDO:C1	2.30	0.42
1:B:62:THR:HA	1:B:174:PHE:O	2.19	0.42
1:A:98:VAL:HG22	1:A:298:LEU:HD23	2.01	0.42
1:A:168:ALA:HB3	1:A:229:PHE:HZ	1.85	0.42
1:B:26:ILE:HD12	1:B:27:ASN:N	2.35	0.42
1:A:186:PHE:CE2	1:A:253:TRP:CD1	3.07	0.42
1:A:275:SER:HA	1:A:276:PRO:HD3	1.90	0.42
1:A:22:THR:O	1:A:25:ILE:HG22	2.20	0.41
1:B:180:ARG:HH22	1:B:185:ASN:CG	2.24	0.41
1:B:39:VAL:O	1:B:39:VAL:HG12	2.21	0.41
4:B:403:NAG:HO3	4:B:403:NAG:C7	2.25	0.41
1:A:36:SER:O	1:A:40:GLY:N	2.54	0.41
1:A:39:VAL:O	1:A:39:VAL:HG12	2.20	0.41
1:A:144:LEU:HD12	1:A:145:ARG:H	1.86	0.41
1:B:38:PHE:CE1	1:B:331:SER:HB3	2.56	0.41
1:B:98:VAL:HG22	1:B:298:LEU:HD23	2.03	0.41
1:B:43:PHE:CD2	1:B:44:LEU:HD23	2.56	0.40
1:A:188:LYS:HE3	1:A:253:TRP:CZ3	2.57	0.40
1:B:132:ILE:O	1:B:149:ILE:HA	2.21	0.40
1:A:107:CYS:HB2	1:A:108:PRO:HD2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:MET:O	1:B:198:ARG:NH2[6_566]	2.15	0.05



## 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	331/363 (91%)	326 (98%)	5 (2%)	0	100	100
1	B	314/363 (86%)	310 (99%)	4 (1%)	0	100	100
All	All	645/726 (89%)	636 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/318 (88%)	277 (99%)	3 (1%)	70	90
1	B	267/318 (84%)	266 (100%)	1 (0%)	89	97
All	All	547/636 (86%)	543 (99%)	4 (1%)	81	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	THR
1	A	292	SER
1	A	308	LEU
1	B	292	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLC	C	1	2	12,12,12	0.51	0	17,17,17	0.56	0
2	GLC	C	2	2	11,11,12	0.60	0	15,15,17	1.06	1 (6%)

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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-C2-C3	2.25	112.91	109.64

There are no chirality outliers.

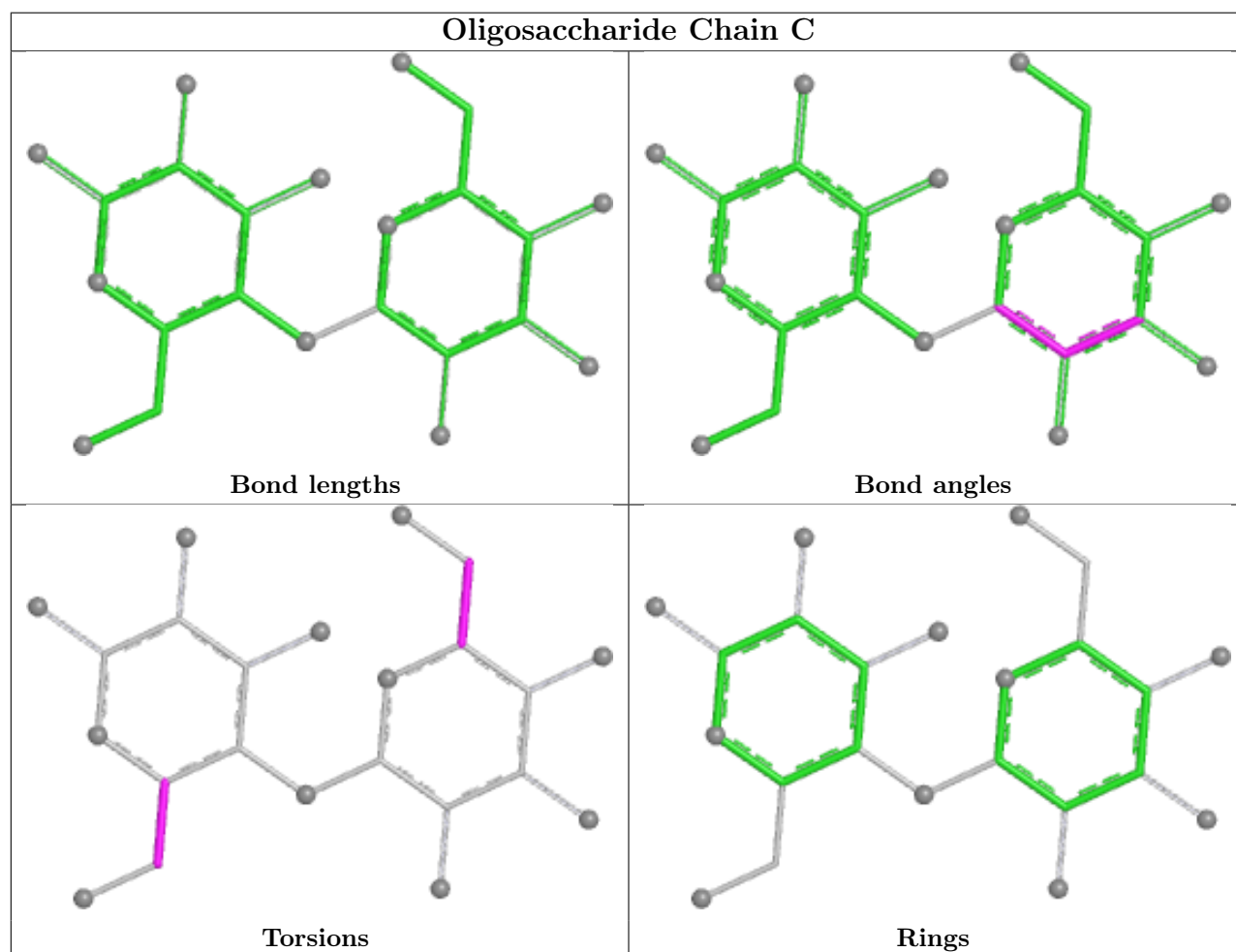
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	GLC	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](#)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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$
4	NAG	A	404	1	14,14,15	1.09	1 (7%)	17,19,21	0.63	0
4	NAG	A	403	1	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	B	404	1	14,14,15	0.37	0	17,19,21	0.59	0
3	ATP	B	401	7	28,33,33	0.90	0	34,52,52	1.12	1 (2%)
3	ATP	A	401	7	28,33,33	1.10	2 (7%)	34,52,52	1.10	2 (5%)
4	NAG	B	402	1	14,14,15	0.92	1 (7%)	17,19,21	1.52	1 (5%)
4	NAG	B	403	1	14,14,15	0.64	0	17,19,21	1.50	4 (23%)
6	ACT	A	411	-	3,3,3	0.87	0	3,3,3	1.45	0
8	TRS	A	414	-	7,7,7	0.30	0	9,9,9	0.22	0
5	EDO	A	406	-	3,3,3	0.77	0	2,2,2	0.44	0
5	EDO	A	409	-	3,3,3	0.75	0	2,2,2	0.42	0
5	EDO	A	408	-	3,3,3	0.74	0	2,2,2	0.48	0
5	EDO	B	405	-	3,3,3	0.74	0	2,2,2	0.53	0
5	EDO	B	406	-	3,3,3	0.62	0	2,2,2	0.91	0
6	ACT	A	410	-	3,3,3	0.79	0	3,3,3	1.41	0
6	ACT	B	407	-	3,3,3	0.92	0	3,3,3	1.35	0
4	NAG	A	402	1	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
5	EDO	A	407	-	3,3,3	0.73	0	2,2,2	0.48	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
4	NAG	A	404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	404	1	-	2/6/23/26	0/1/1/1
3	ATP	B	401	7	-	3/18/38/38	0/3/3/3
3	ATP	A	401	7	-	3/18/38/38	0/3/3/3
4	NAG	B	402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	403	1	-	2/6/23/26	0/1/1/1
8	TRS	A	414	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	406	-	-	0/1/1/1	-
5	EDO	A	409	-	-	1/1/1/1	-
5	EDO	A	408	-	-	0/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	EDO	A	407	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	NAG	O5-C1	-3.93	1.37	1.43
4	B	402	NAG	O5-C1	3.37	1.49	1.43
3	A	401	ATP	PB-O3A	2.53	1.62	1.59
3	A	401	ATP	PA-O3A	2.51	1.62	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	NAG	C1-O5-C5	6.03	120.27	112.19
3	B	401	ATP	N3-C2-N1	-4.21	122.96	128.67
3	A	401	ATP	N3-C2-N1	-3.44	124.01	128.67
4	B	403	NAG	C8-C7-N2	3.40	121.75	116.12
4	B	403	NAG	C1-C2-N2	2.91	115.03	110.43
4	A	402	NAG	C1-O5-C5	2.45	115.47	112.19
3	A	401	ATP	N6-C6-N1	2.10	122.82	118.33
4	B	403	NAG	O7-C7-N2	-2.08	118.31	121.98
4	B	403	NAG	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	NAG	O5-C5-C6-O6
4	B	402	NAG	C4-C5-C6-O6
4	A	404	NAG	O5-C5-C6-O6
4	B	404	NAG	O5-C5-C6-O6
4	A	403	NAG	O5-C5-C6-O6
5	A	409	EDO	O1-C1-C2-O2
4	A	404	NAG	C4-C5-C6-O6
4	B	403	NAG	O5-C5-C6-O6

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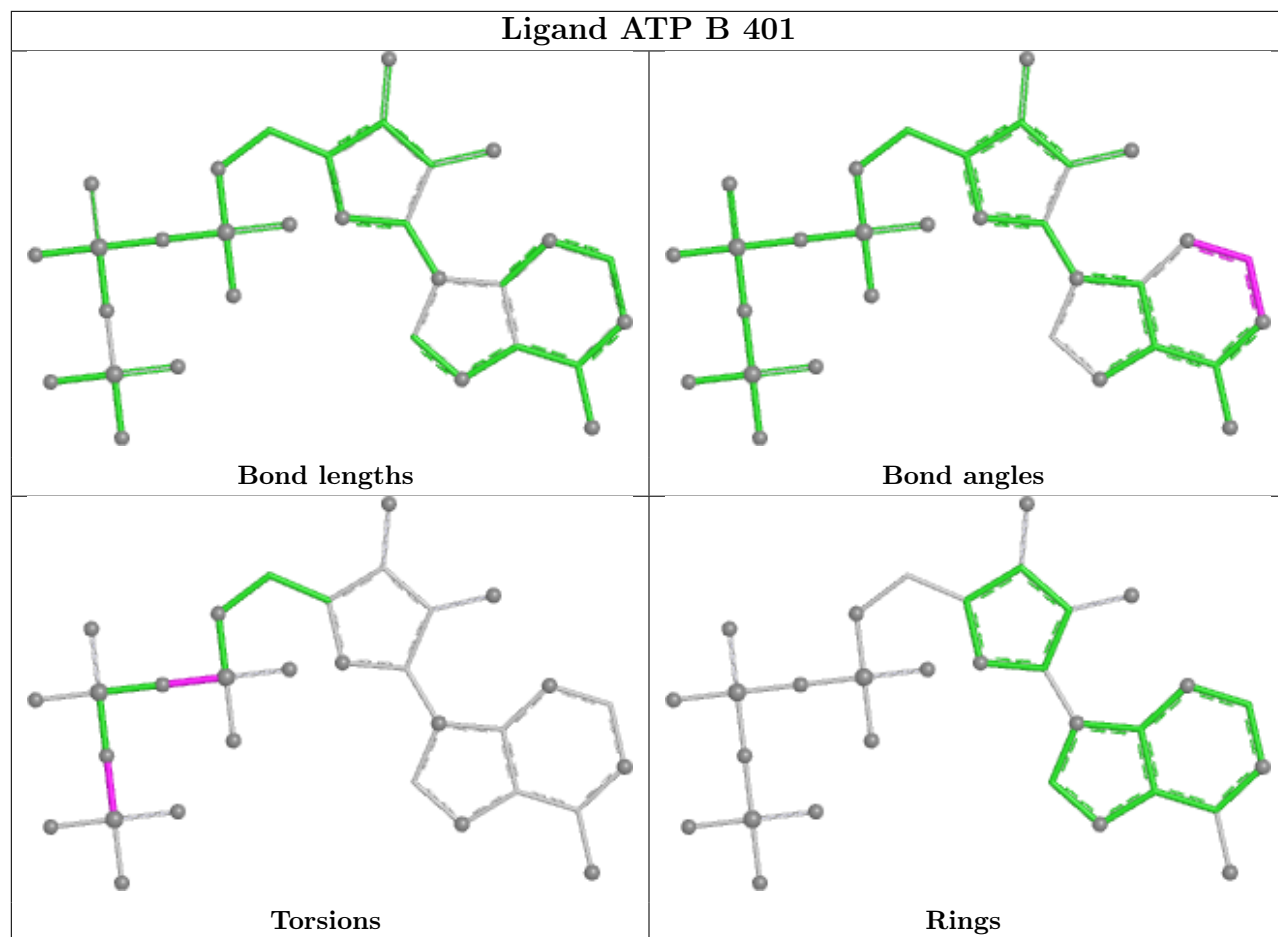
Mol	Chain	Res	Type	Atoms
4	B	404	NAG	C4-C5-C6-O6
4	B	403	NAG	C3-C2-N2-C7
3	A	401	ATP	PB-O3B-PG-O1G
3	B	401	ATP	PB-O3A-PA-O1A
4	A	403	NAG	C4-C5-C6-O6
3	A	401	ATP	PB-O3B-PG-O2G
3	A	401	ATP	PB-O3B-PG-O3G
3	B	401	ATP	PB-O3B-PG-O3G
3	B	401	ATP	PB-O3B-PG-O1G

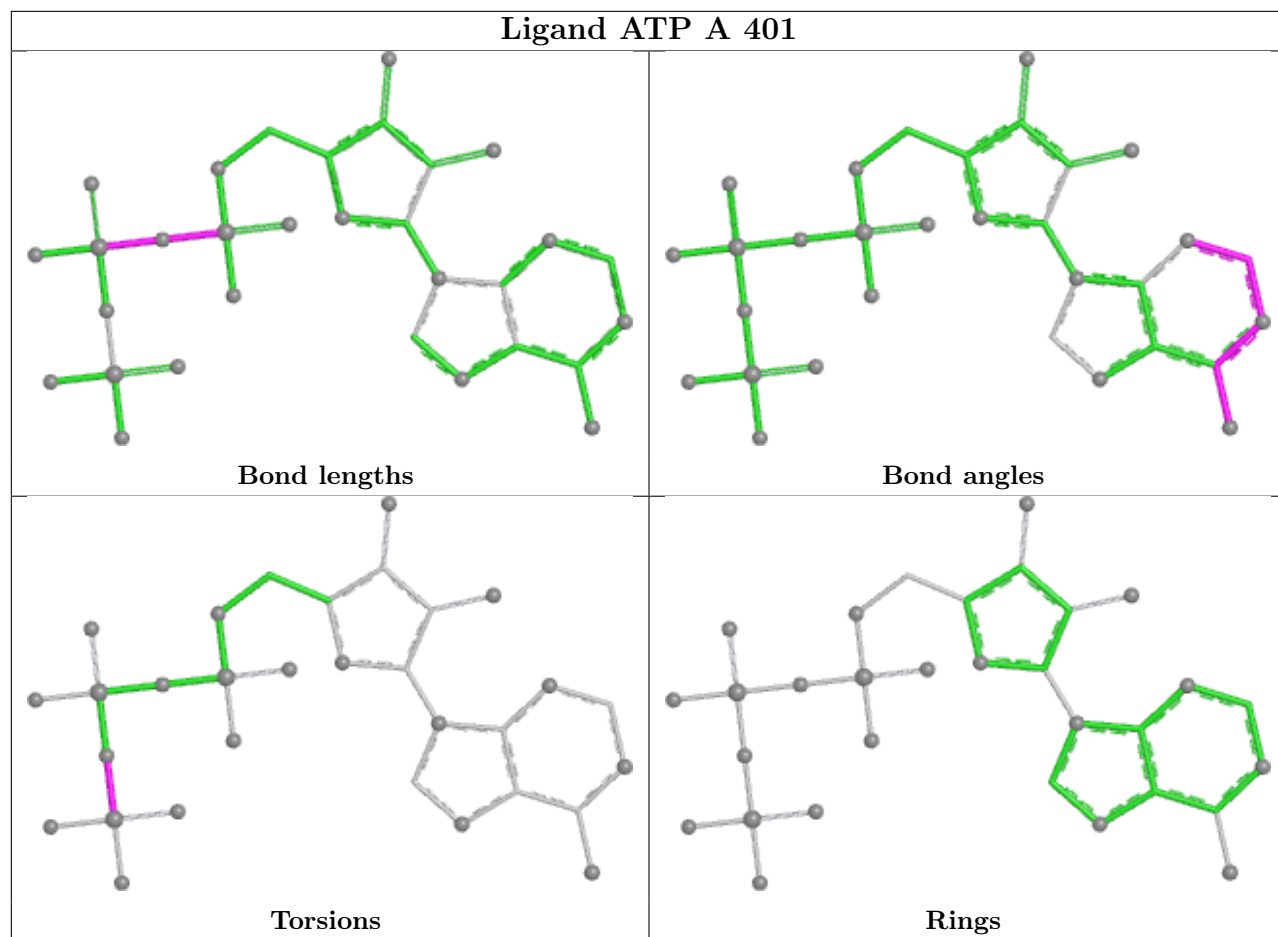
There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ATP	2	0
3	A	401	ATP	2	0
4	B	403	NAG	2	0
5	A	409	EDO	3	0
5	A	408	EDO	3	0
5	B	406	EDO	2	0
4	A	402	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/363 (91%)	0.67	43 (12%) 9 7	51, 79, 144, 170	0
1	B	318/363 (87%)	0.66	43 (13%) 8 7	52, 83, 146, 155	0
All	All	651/726 (89%)	0.67	86 (13%) 8 7	51, 80, 145, 170	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	PRO	7.0
1	A	72	ASN	7.0
1	A	120	SER	6.5
1	B	255	GLN	6.3
1	A	121	GLN	5.9
1	B	120	SER	5.9
1	B	344	LEU	5.7
1	A	344	LEU	5.7
1	B	285	TYR	5.6
1	B	123	GLY	5.6
1	B	286	TYR	5.4
1	A	23	ILE	5.1
1	A	338	LEU	4.6
1	B	284	LYS	4.6
1	A	17	VAL	4.6
1	B	345	ASN	4.1
1	B	130	GLY	4.0
1	A	193	PRO	3.9
1	B	273	SER	3.9
1	A	22	THR	3.8
1	A	343	LEU	3.8
1	A	14	LYS	3.7
1	A	89	VAL	3.7
1	B	126	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	273	SER	3.6
1	B	32	LEU	3.6
1	A	130	GLY	3.5
1	B	253	TRP	3.4
1	A	20	SER	3.4
1	A	85	GLN	3.4
1	B	283	ALA	3.4
1	B	44	LEU	3.3
1	B	343	LEU	3.3
1	B	158	ASP	3.3
1	A	271	LYS	3.3
1	B	113	LYS	3.3
1	A	346	PHE	3.2
1	A	18	VAL	3.1
1	B	139	ASN	3.1
1	A	334	VAL	3.1
1	A	122	CYS	3.1
1	B	41	TRP	3.0
1	B	316	PHE	3.0
1	A	15	SER	3.0
1	A	342	ILE	3.0
1	B	159	THR	3.0
1	B	329	PHE	2.9
1	A	35	ILE	2.9
1	B	26	ILE	2.9
1	B	125	GLU	2.9
1	B	252	ALA	2.8
1	B	234	ARG	2.8
1	A	341	ILE	2.8
1	A	123	GLY	2.7
1	A	277	GLY	2.7
1	A	337	VAL	2.6
1	B	118	SER	2.6
1	A	198	ARG	2.6
1	B	272	SER	2.5
1	A	126	ARG	2.5
1	B	73	ARG	2.5
1	B	114	TYR	2.5
1	A	282	PHE	2.4
1	A	21	TRP	2.4
1	B	290	ASN	2.4
1	B	245	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	2.4
1	A	201	LYS	2.4
1	A	283	ALA	2.4
1	A	124	PRO	2.3
1	B	330	THR	2.3
1	A	82	THR	2.3
1	B	38	PHE	2.3
1	B	306	ASP	2.3
1	A	127	LEU	2.2
1	A	335	GLY	2.2
1	A	318	ILE	2.2
1	B	143	VAL	2.2
1	A	118	SER	2.1
1	A	51	VAL	2.1
1	B	145	ARG	2.1
1	A	87	THR	2.1
1	B	31	GLN	2.1
1	B	254	ASP	2.0
1	B	289	GLU	2.0
1	A	83	PRO	2.0

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

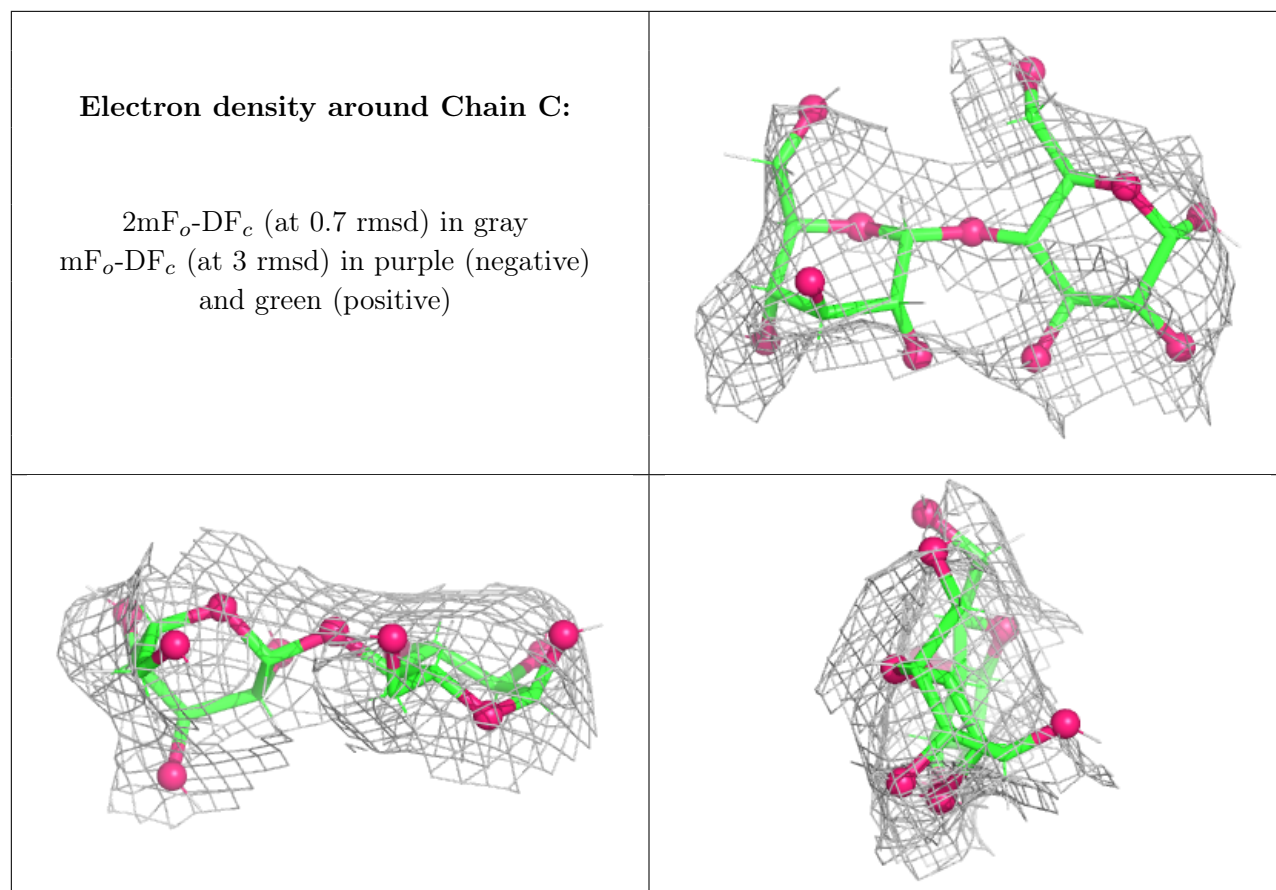
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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
2	GLC	C	1	12/12	0.28	0.18	149,189,227,229	0
2	GLC	C	2	11/12	0.57	0.18	150,195,228,235	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	404	14/15	0.64	0.17	108,145,173,177	0
5	EDO	A	408	4/4	0.64	0.21	115,118,121,123	0
6	ACT	A	411	4/4	0.72	0.36	96,103,104,112	0
4	NAG	B	402	14/15	0.74	0.13	83,120,146,156	0
4	NAG	B	403	14/15	0.77	0.18	78,100,123,151	0
6	ACT	A	410	4/4	0.78	0.32	103,117,119,126	0
4	NAG	A	404	14/15	0.79	0.12	105,126,149,152	0
7	NA	A	413	1/1	0.79	0.25	102,102,102,102	0
5	EDO	B	405	4/4	0.80	0.38	90,99,110,111	0
6	ACT	B	407	4/4	0.81	0.26	80,88,101,101	0
5	EDO	A	406	4/4	0.87	0.28	73,88,90,98	0
5	EDO	A	407	4/4	0.88	0.37	109,113,116,119	0
4	NAG	A	403	14/15	0.89	0.09	78,100,123,151	0

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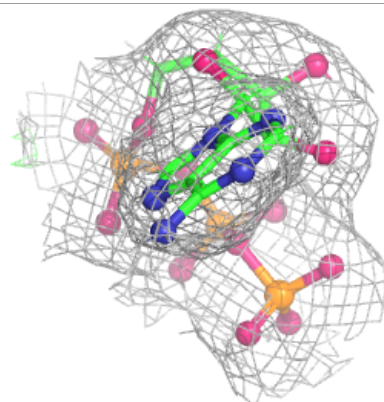
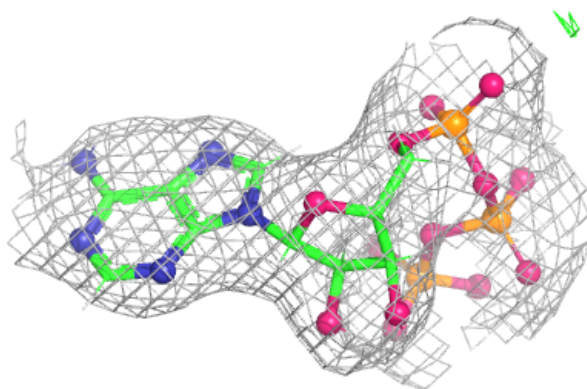
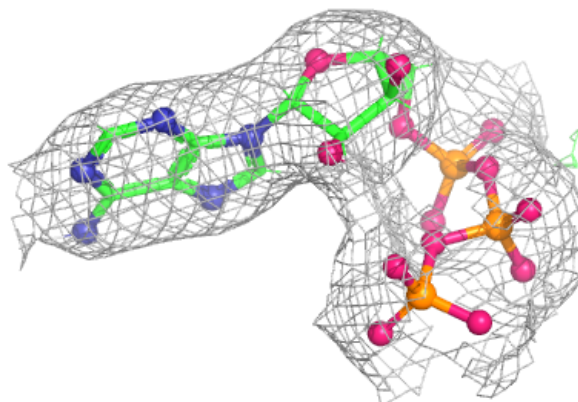
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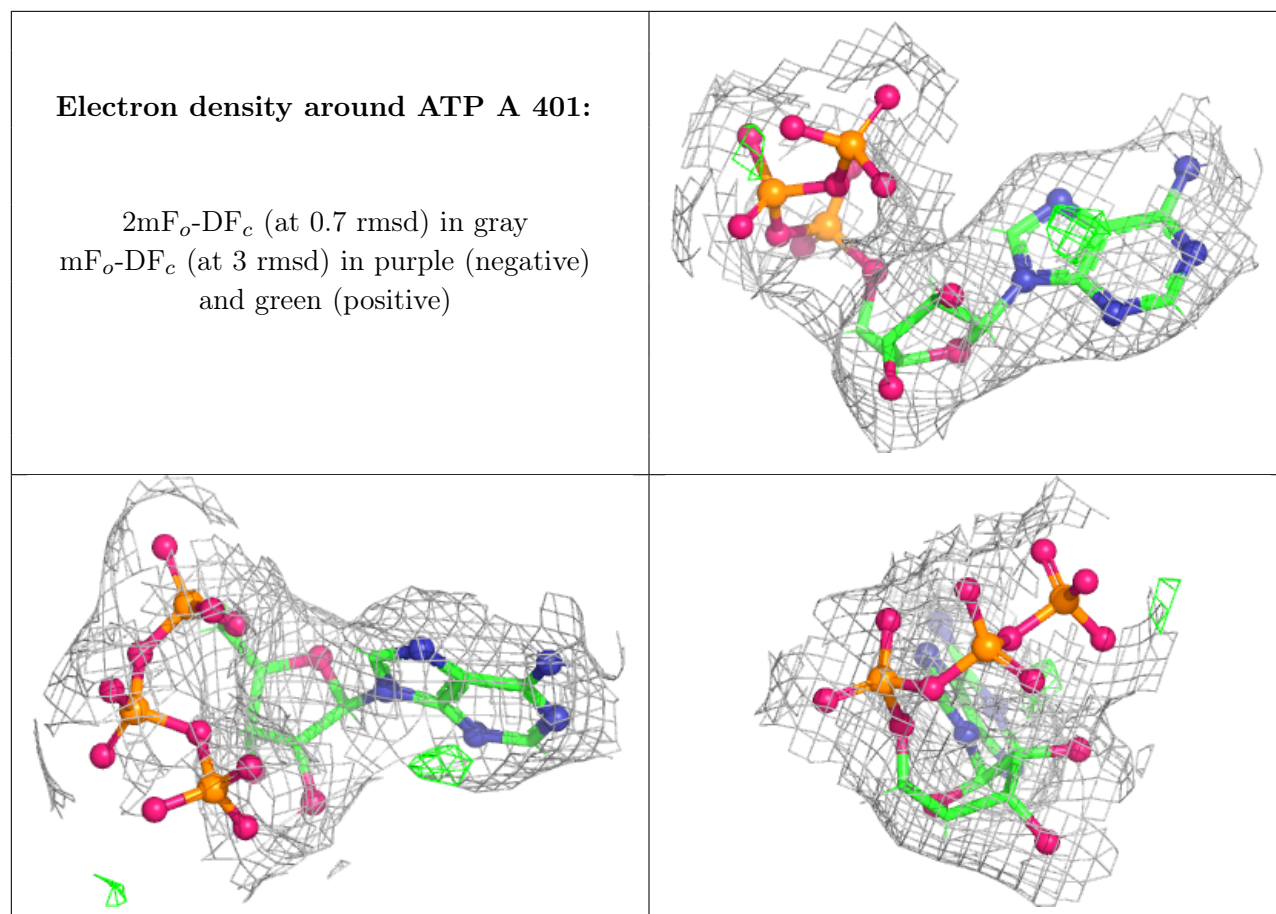
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NA	B	408	1/1	0.90	0.22	103,103,103,103	0
8	TRS	A	414	8/8	0.94	0.12	137,142,147,149	8
5	EDO	B	406	4/4	0.95	0.15	64,68,75,88	0
5	EDO	A	409	4/4	0.95	0.16	56,73,80,88	0
7	NA	A	412	1/1	0.95	0.10	76,76,76,76	0
4	NAG	A	402	14/15	0.96	0.08	52,69,103,113	0
3	ATP	B	401	31/31	0.98	0.06	54,64,79,122	0
3	ATP	A	401	31/31	0.98	0.06	49,64,82,112	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 ATP B 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.