



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:47 PM BST

PDB ID : 5U2H
Title : Crystal structure of the ATP-gated P2X7 ion channel bound to ATP and allosteric antagonist A804598
Authors : Karasawa, A.; Kawate, T.
Deposited on : 2016-11-30
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

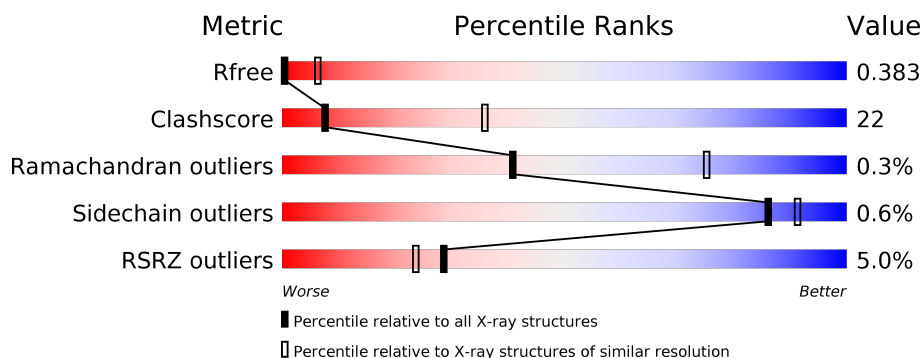
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>10%</div> </div> </div>
1	B	342	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>13%</div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	7S1	A	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4184 atoms, of which 68 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2022	1276	336	396	14			
1	B	299	Total	C	N	O	S	0	0	0
			1945	1222	325	386	12			

There are 22 discrepancies between the modelled and reference sequences:

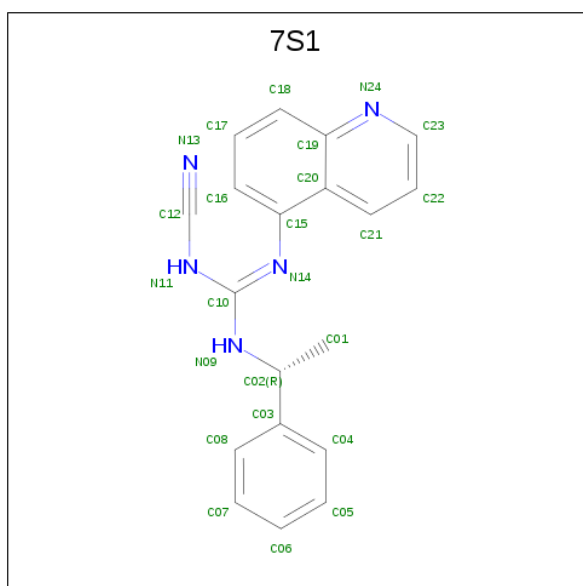
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP G1M6C4
A	22	SER	-	expression tag	UNP G1M6C4
A	35	ALA	VAL	engineered mutation	UNP G1M6C4
A	125	ALA	ARG	engineered mutation	UNP G1M6C4
A	174	LYS	GLU	engineered mutation	UNP G1M6C4
A	241	SER	ASN	engineered mutation	UNP G1M6C4
A	284	SER	ASN	engineered mutation	UNP G1M6C4
A	359	SER	-	expression tag	UNP G1M6C4
A	360	ALA	-	expression tag	UNP G1M6C4
A	361	SER	-	expression tag	UNP G1M6C4
A	362	SER	-	expression tag	UNP G1M6C4
B	21	GLY	-	expression tag	UNP G1M6C4
B	22	SER	-	expression tag	UNP G1M6C4
B	35	ALA	VAL	engineered mutation	UNP G1M6C4
B	125	ALA	ARG	engineered mutation	UNP G1M6C4
B	174	LYS	GLU	engineered mutation	UNP G1M6C4
B	241	SER	ASN	engineered mutation	UNP G1M6C4
B	284	SER	ASN	engineered mutation	UNP G1M6C4
B	359	SER	-	expression tag	UNP G1M6C4
B	360	ALA	-	expression tag	UNP G1M6C4
B	361	SER	-	expression tag	UNP G1M6C4
B	362	SER	-	expression tag	UNP G1M6C4

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



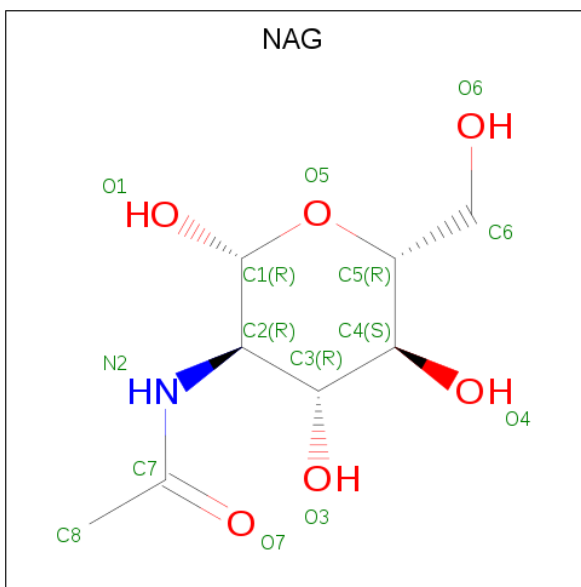
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 3 is N-cyano-N'-[(1R)-1-phenylethyl]-N''-quinolin-5-ylguanidine (three-letter code: 7S1) (formula: C₁₉H₁₇N₅).



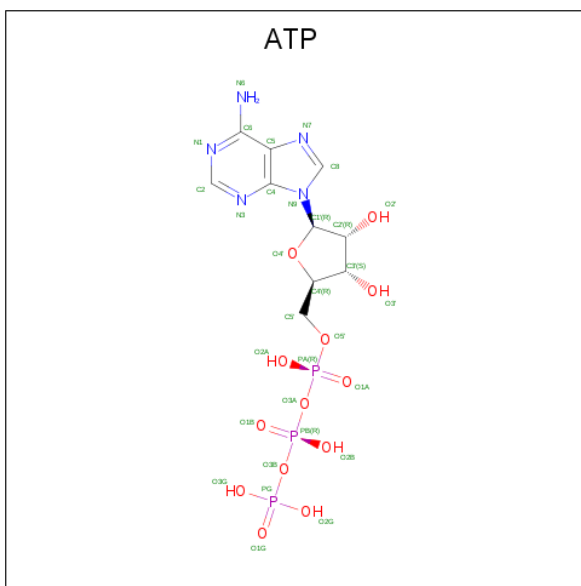
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			24	19	5		
3	B	1	Total	C	N	0	0
			24	19	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

Chain C:  50% 50%

MAC1
MAC2

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

Chain D:  100%

MAC1
MAC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	167.62Å 167.62Å 167.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.90 48.39 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.39-3.90) 100.0 (48.39-3.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.334 , 0.386 0.331 , 0.383	Depositor DCC
R_{free} test set	1445 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	150.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	4184	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.26% 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: 7S1, NAG, ATP

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	0.24	0/2062	0.42	0/2832
1	B	0.24	0/1980	0.41	0/2720
All	All	0.24	0/4042	0.41	0/5552

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	2022	0	1595	83	0
1	B	1945	0	1524	75	1
2	C	28	27	25	1	0
2	D	28	27	25	0	0
3	A	24	0	0	1	0
3	B	24	0	0	1	0
4	B	14	14	13	0	0
5	B	31	0	12	1	0
All	All	4116	68	3194	161	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 22.

All (161) 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:A:53:LYS:O	1:A:326:GLY:HA2	1.38	1.20
1:A:252:MET:O	1:A:317:PHE:HA	1.62	0.98
1:A:250:GLY:O	1:A:315:ILE:HA	1.70	0.92
1:A:164:VAL:HG21	1:A:170:ILE:HD11	1.56	0.88
1:A:292:ASN:HA	1:A:312:VAL:O	1.78	0.83
1:A:185:ALA:HB3	1:A:242:PHE:HZ	1.42	0.83
1:B:59:SER:HA	1:B:195:ASN:O	1.80	0.82
1:B:185:ALA:HB3	1:B:242:PHE:HZ	1.48	0.79
1:A:54:LYS:HA	1:A:325:GLY:O	1.83	0.78
1:B:185:ALA:HB3	1:B:242:PHE:CZ	2.19	0.78
1:A:120:PRO:HB3	1:A:153:VAL:HG23	1.66	0.76
1:A:132:ASP:HA	1:A:152:CYS:HB3	1.67	0.76
1:B:186:GLU:HB3	1:B:242:PHE:CG	2.21	0.75
1:B:250:GLY:O	1:B:315:ILE:HA	1.85	0.75
1:B:67:GLY:O	1:B:93:TYR:OH	2.02	0.75
1:A:67:GLY:O	1:A:93:TYR:OH	2.05	0.73
1:B:252:MET:O	1:B:317:PHE:HA	1.90	0.72
1:B:71:VAL:O	1:B:85:SER:HA	1.90	0.72
1:A:107:ASN:HD21	1:A:177:PRO:HG2	1.56	0.69
1:B:106:THR:HB	1:B:246:ALA:HB1	1.74	0.69
1:A:123:PRO:HD3	1:A:155:TYR:CD2	2.27	0.69
1:B:107:ASN:HD21	1:B:177:PRO:HG2	1.56	0.69
1:B:172:GLU:OE1	1:B:174:LYS:NZ	2.26	0.69
1:A:129:CYS:HB3	1:A:135:CYS:SG	2.33	0.68
1:B:78:ASN:HA	1:B:172:GLU:OE2	1.94	0.68
1:B:65:VAL:HB	1:B:90:THR:HG23	1.76	0.67
1:A:235:PHE:HA	1:A:238:THR:HG22	1.77	0.67
1:B:235:PHE:HB3	1:B:240:ASP:O	1.95	0.66
1:B:124:THR:N	1:B:127:THR:OG1	2.28	0.66
1:B:240:ASP:OD2	1:B:277:ARG:HD3	1.96	0.66
1:B:243:SER:O	1:B:247:ILE:HG13	1.97	0.65
1:A:122:PHE:CD1	1:A:123:PRO:HD2	2.32	0.64
1:A:186:GLU:HB3	1:A:242:PHE:CD2	2.32	0.64
1:A:90:THR:O	1:A:94:THR:HG22	1.97	0.64
1:A:296:ALA:HB2	1:A:309:LEU:HD12	1.80	0.62
1:B:185:ALA:HA	1:B:188:PHE:CD2	2.35	0.62
1:A:52:GLN:HA	1:A:328:PHE:HA	1.82	0.62
1:B:121:ASP:OD1	1:B:122:PHE:N	2.33	0.61
1:A:219:HIS:HB3	1:A:223:ASN:H	1.64	0.61
1:A:69:ALA:CB	1:A:184:SER:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HA	1:B:193:LYS:O	2.01	0.60
1:B:251:ILE:HD11	1:B:291:TYR:HD2	1.66	0.60
5:B:405:ATP:O3A	5:B:405:ATP:H3'	2.02	0.60
1:A:121:ASP:OD1	1:A:122:PHE:N	2.34	0.59
1:B:65:VAL:HG11	1:B:93:TYR:HE1	1.68	0.59
1:A:124:THR:N	1:A:127:THR:OG1	2.34	0.59
1:A:57:LEU:HD23	1:A:58:ILE:N	2.17	0.58
1:B:191:LEU:HD13	1:B:228:ILE:HD11	1.84	0.58
1:A:71:VAL:HG22	1:A:181:LEU:O	2.03	0.58
1:B:255:GLU:HG3	1:B:274:SER:OG	2.03	0.58
1:A:105:MET:O	1:A:182:LEU:HD23	2.03	0.58
1:A:235:PHE:CE1	1:A:252:MET:HG3	2.39	0.58
1:B:256:ILE:HA	1:B:272:LYS:O	2.03	0.58
1:B:235:PHE:HZ	1:B:315:ILE:HD13	1.69	0.57
1:B:107:ASN:ND2	1:B:177:PRO:HG2	2.19	0.57
1:B:164:VAL:HG21	1:B:170:ILE:HD11	1.84	0.57
1:A:121:ASP:HA	1:A:170:ILE:HD12	1.86	0.57
1:B:124:THR:O	1:B:128:ILE:HG12	2.04	0.56
1:B:69:ALA:HB2	1:B:188:PHE:CZ	2.39	0.56
1:A:124:THR:HG22	1:A:125:ALA:H	1.68	0.56
1:B:124:THR:HG22	1:B:125:ALA:H	1.69	0.56
1:B:249:GLY:O	1:B:290:GLY:HA2	2.06	0.56
1:B:164:VAL:CG2	1:B:170:ILE:HD11	2.37	0.55
1:A:123:PRO:HD3	1:A:155:TYR:HD2	1.70	0.55
1:A:120:PRO:HB3	1:A:153:VAL:CG2	2.37	0.55
1:A:122:PHE:CG	1:A:123:PRO:HD2	2.43	0.54
1:B:121:ASP:HA	1:B:170:ILE:HD12	1.89	0.54
1:B:59:SER:OG	1:B:194:ASN:OD1	2.20	0.54
1:A:185:ALA:HB3	1:A:242:PHE:CZ	2.32	0.54
1:A:157:GLU:HA	1:A:157:GLU:OE1	2.08	0.54
1:B:245:VAL:HG13	1:B:250:GLY:HA3	1.90	0.54
1:B:251:ILE:HB	1:B:279:ASP:CB	2.38	0.54
1:A:65:VAL:HG11	1:A:93:TYR:HE1	1.74	0.53
1:B:69:ALA:HB2	1:B:188:PHE:HZ	1.73	0.52
1:B:277:ARG:CZ	1:B:282:THR:HA	2.40	0.52
1:A:69:ALA:HB2	1:A:184:SER:HB2	1.91	0.52
1:B:234:ILE:HG12	1:B:275:PHE:CE2	2.45	0.52
1:B:74:GLU:O	1:B:75:ILE:HD13	2.09	0.51
1:A:218:PHE:HB2	1:A:226:CYS:O	2.11	0.51
1:A:291:TYR:HB3	1:A:314:GLY:O	2.11	0.51
1:B:288:TYR:N	1:B:289:PRO:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:CYS:HA	1:A:268:HIS:O	2.11	0.50
1:B:177:PRO:O	1:B:247:ILE:HG23	2.11	0.50
1:A:124:THR:HG22	1:A:125:ALA:N	2.26	0.50
1:B:63:THR:HA	1:B:191:LEU:O	2.11	0.50
1:A:280:ASP:O	1:A:281:LYS:HB2	2.12	0.50
1:B:89:ASP:OD1	1:B:91:ALA:N	2.44	0.50
1:B:209:LEU:N	1:B:210:PRO:HD2	2.27	0.50
1:B:124:THR:HG22	1:B:125:ALA:N	2.27	0.50
1:A:119:CYS:O	1:A:164:VAL:HG22	2.12	0.50
1:A:235:PHE:HB3	1:A:240:ASP:O	2.12	0.50
3:B:404:7S1:C12	3:B:404:7S1:C02	2.90	0.49
1:A:135:CYS:HB3	1:A:148:GLN:OE1	2.11	0.49
1:A:132:ASP:HA	1:A:152:CYS:CB	2.40	0.49
1:A:235:PHE:CE2	1:A:242:PHE:HD1	2.31	0.49
1:A:283:THR:CB	1:A:289:PRO:HG3	2.42	0.49
1:A:118:LEU:CD2	1:A:165:SER:HB2	2.43	0.49
1:B:90:THR:O	1:B:94:THR:HG22	2.12	0.48
1:A:105:MET:HG2	1:A:182:LEU:HD22	1.96	0.48
1:B:277:ARG:HH21	1:B:280:ASP:CB	2.27	0.48
1:A:123:PRO:HD3	1:A:155:TYR:CE2	2.48	0.48
1:B:123:PRO:HA	1:B:161:THR:HG21	1.95	0.48
1:A:262:LEU:N	1:A:326:GLY:O	2.43	0.48
3:A:403:7S1:C02	3:A:403:7S1:C12	2.92	0.48
1:A:183:ASN:OD1	1:A:184:SER:N	2.47	0.47
1:A:235:PHE:HA	1:A:238:THR:CG2	2.44	0.47
1:B:186:GLU:HB3	1:B:242:PHE:CD2	2.49	0.47
1:B:195:ASN:HA	1:B:206:ARG:CB	2.45	0.47
1:A:153:VAL:O	1:A:160:LYS:HA	2.15	0.47
1:A:76:LEU:HA	1:A:81:LYS:HA	1.97	0.47
1:A:235:PHE:CZ	1:A:315:ILE:HD13	2.50	0.47
1:A:186:GLU:HB3	1:A:242:PHE:CE2	2.50	0.46
1:B:107:ASN:OD1	1:B:181:LEU:HG	2.15	0.46
1:B:191:LEU:HD13	1:B:228:ILE:CD1	2.46	0.46
1:A:235:PHE:HE1	1:A:252:MET:HG3	1.80	0.46
1:A:258:TRP:HB2	1:A:323:GLY:CA	2.46	0.46
1:A:292:ASN:CA	1:A:312:VAL:O	2.58	0.46
1:B:172:GLU:HB2	1:B:174:LYS:NZ	2.31	0.46
1:A:186:GLU:HG3	1:A:187:ASN:N	2.31	0.45
1:A:57:LEU:HD21	1:A:196:ILE:CB	2.47	0.45
1:A:184:SER:HA	2:C:1:NAG:C8	2.47	0.45
1:B:102:PHE:CZ	1:B:190:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HA	1:B:231:LEU:CB	2.47	0.45
1:B:135:CYS:SG	1:B:148:GLN:HB3	2.57	0.45
1:B:237:GLU:HG3	1:B:275:PHE:CD1	2.51	0.45
1:A:234:ILE:HG12	1:A:275:PHE:CE2	2.51	0.45
1:B:190:VAL:CG1	1:B:229:PHE:HB2	2.46	0.45
1:A:232:GLY:O	1:A:236:GLN:HG3	2.17	0.45
1:B:229:PHE:HZ	1:B:273:TYR:CE2	2.35	0.45
1:A:176:ALA:HB3	1:A:247:ILE:HG22	1.98	0.44
1:A:71:VAL:O	1:A:85:SER:HA	2.17	0.44
1:A:240:ASP:OD2	1:A:281:LYS:HE2	2.17	0.44
1:A:258:TRP:HB2	1:A:323:GLY:HA2	1.99	0.44
1:A:230:ARG:HD3	1:A:233:ASP:OD1	2.17	0.44
1:B:299:TYR:HE2	1:B:308:THR:OG1	2.01	0.44
1:A:296:ALA:HA	1:A:308:THR:O	2.18	0.44
1:B:189:THR:HB	1:B:228:ILE:CG2	2.48	0.43
1:A:95:PHE:HB3	1:A:96:PRO:HD2	2.00	0.43
1:B:235:PHE:CZ	1:B:315:ILE:HD13	2.52	0.43
1:A:106:THR:HB	1:A:246:ALA:HB1	1.99	0.43
1:B:157:GLU:OE1	1:B:157:GLU:HA	2.19	0.43
1:B:337:ILE:O	1:B:341:ILE:CB	2.66	0.43
1:A:177:PRO:O	1:A:247:ILE:HG23	2.19	0.43
1:A:189:THR:HB	1:A:228:ILE:HG22	2.00	0.43
1:A:107:ASN:ND2	1:A:177:PRO:HG2	2.29	0.42
1:B:245:VAL:CG1	1:B:250:GLY:HA3	2.49	0.42
1:A:235:PHE:HD2	1:A:242:PHE:HB2	1.84	0.42
1:A:185:ALA:HA	1:A:188:PHE:CE2	2.53	0.42
1:A:258:TRP:CZ2	1:A:271:PRO:HB3	2.54	0.42
1:A:106:THR:HA	1:A:182:LEU:HB2	2.02	0.42
1:B:296:ALA:HA	1:B:308:THR:O	2.20	0.42
1:B:235:PHE:CE2	1:B:242:PHE:HD1	2.38	0.42
1:B:291:TYR:HE2	1:B:316:ARG:HH21	1.66	0.42
1:B:204:THR:HG22	1:B:205:THR:N	2.35	0.42
1:A:251:ILE:HD11	1:A:291:TYR:HD1	1.85	0.41
1:A:235:PHE:HZ	1:A:315:ILE:HD13	1.85	0.41
1:B:103:PHE:CE1	1:B:314:GLY:HA3	2.55	0.41
1:A:59:SER:HB3	1:A:321:VAL:HG11	2.02	0.41
1:B:135:CYS:SG	1:B:136:LYS:N	2.94	0.41
1:B:122:PHE:CE2	1:B:173:VAL:HB	2.55	0.41
1:B:234:ILE:O	1:B:238:THR:HG22	2.22	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:B:92:ASP:OD1	1:B:298:TYR:OH[5_555]	2.14	0.06

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	301/342 (88%)	290 (96%)	10 (3%)	1 (0%)	41	75
1	B	293/342 (86%)	278 (95%)	14 (5%)	1 (0%)	41	75
All	All	594/684 (87%)	568 (96%)	24 (4%)	2 (0%)	41	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ALA
1	B	166	ALA

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	160/300 (53%)	159 (99%)	1 (1%)	86	91
1	B	151/300 (50%)	150 (99%)	1 (1%)	84	90
All	All	311/600 (52%)	309 (99%)	2 (1%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	TYR
1	B	152	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	C	2	2	14,14,15	0.17	0	17,19,21	0.42	0
2	NAG	D	1	1,2	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	D	2	2	14,14,15	0.19	0	17,19,21	0.40	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

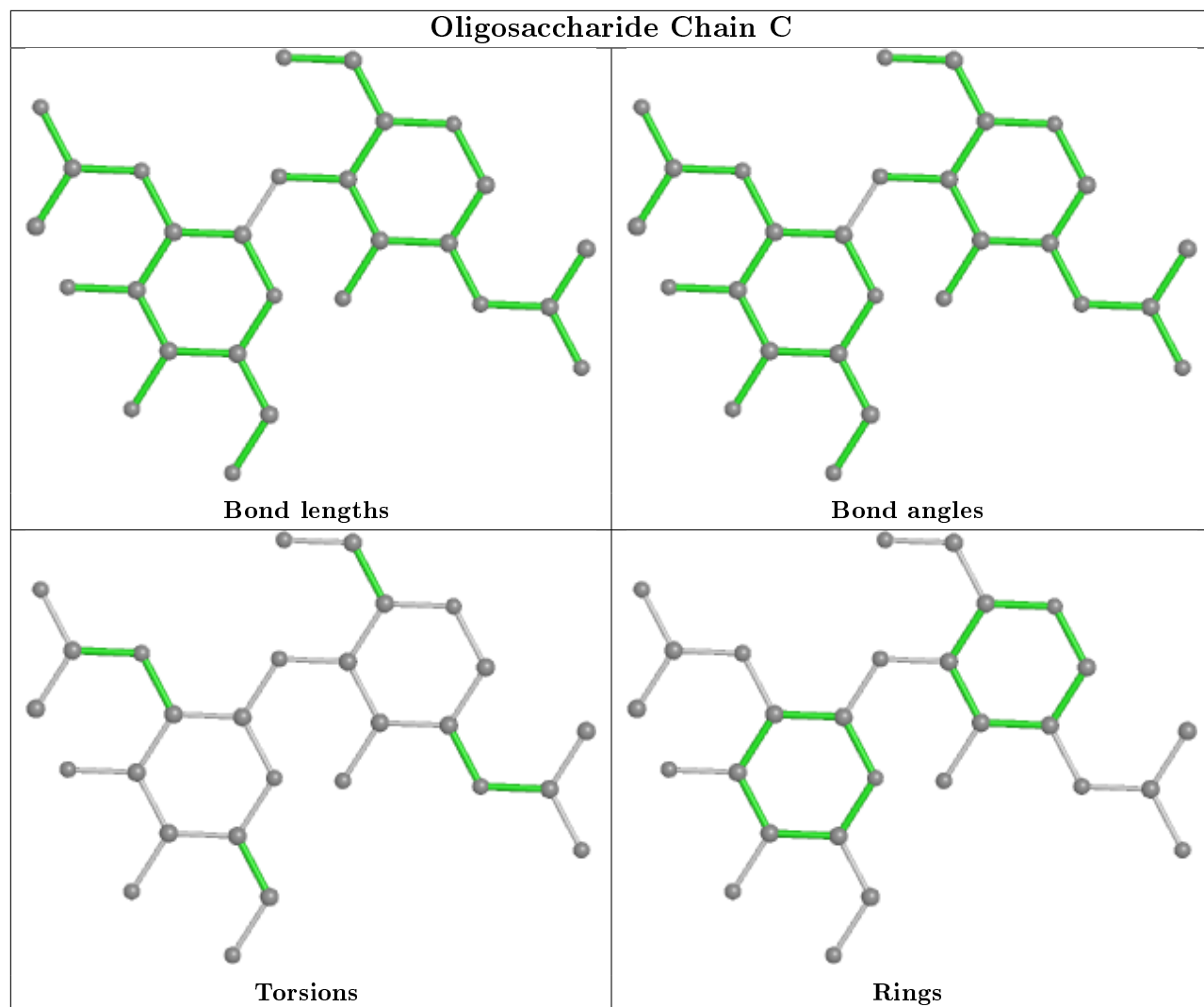
There are no torsion outliers.

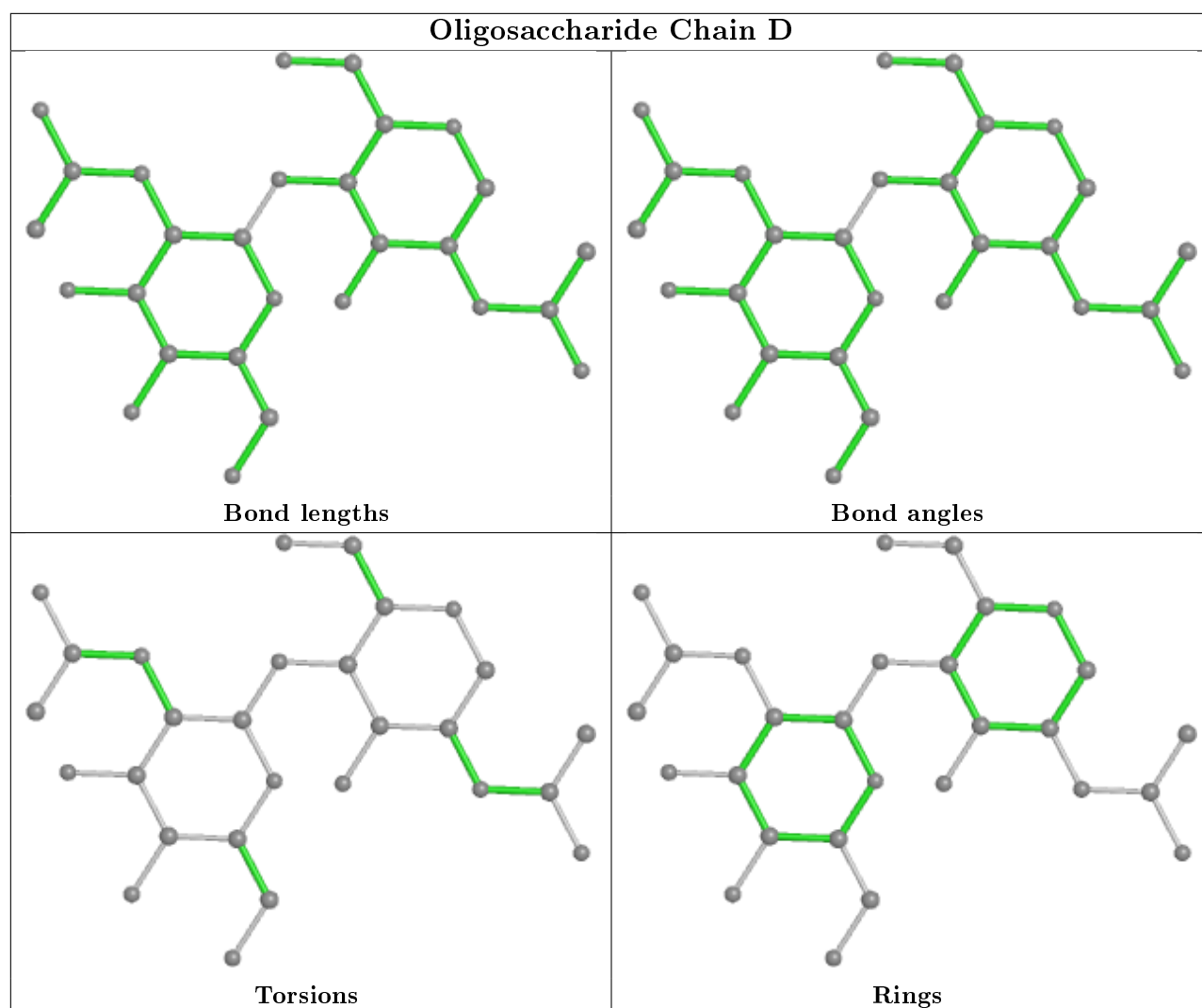
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	7S1	B	404	-	25,26,26	2.90	5 (20%)	30,34,34	1.32	4 (13%)
4	NAG	B	403	1	14,14,15	0.21	0	17,19,21	0.45	0
3	7S1	A	403	-	25,26,26	2.87	6 (24%)	30,34,34	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	B	405	-	26,33,33	0.94	1 (3%)	31,52,52	1.52	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7S1	B	404	-	-	0/12/15/15	0/3/3/3
4	NAG	B	403	1	-	0/6/23/26	0/1/1/1
3	7S1	A	403	-	-	0/12/15/15	0/3/3/3
5	ATP	B	405	-	-	1/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	7S1	C10-N11	9.34	1.48	1.37
3	A	403	7S1	C10-N11	9.17	1.48	1.37
3	A	403	7S1	C10-N14	7.02	1.49	1.31
3	B	404	7S1	C10-N14	6.98	1.49	1.31
3	B	404	7S1	C15-N14	5.33	1.49	1.41
3	A	403	7S1	C15-N14	5.25	1.49	1.41
3	B	404	7S1	C20-C19	-3.22	1.37	1.42
3	A	403	7S1	C20-C19	-3.19	1.37	1.42
3	B	404	7S1	C10-N09	-3.17	1.29	1.35
3	A	403	7S1	C10-N09	-3.12	1.29	1.35
5	B	405	ATP	C5-C4	2.48	1.47	1.40
3	A	403	7S1	C23-N24	2.03	1.36	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	7S1	N11-C10-N09	3.83	125.68	116.78
3	B	404	7S1	N11-C10-N09	3.81	125.64	116.78
5	B	405	ATP	PB-O3B-PG	-3.26	121.64	132.83
5	B	405	ATP	C3'-C2'-C1'	3.20	105.80	100.98
5	B	405	ATP	N3-C2-N1	-3.14	123.76	128.68
5	B	405	ATP	PA-O3A-PB	-2.78	123.30	132.83
3	A	403	7S1	C21-C20-C15	-2.71	120.03	123.23
3	B	404	7S1	C21-C20-C15	-2.66	120.08	123.23
5	B	405	ATP	C4-C5-N7	-2.61	106.68	109.40
3	A	403	7S1	C22-C23-N24	-2.50	120.11	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	7S1	C22-C23-N24	-2.41	120.25	123.94
3	A	403	7S1	C20-C19-N24	-2.38	120.30	122.83
3	B	404	7S1	C20-C19-N24	-2.35	120.33	122.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	405	ATP	PA-O3A-PB-O1B

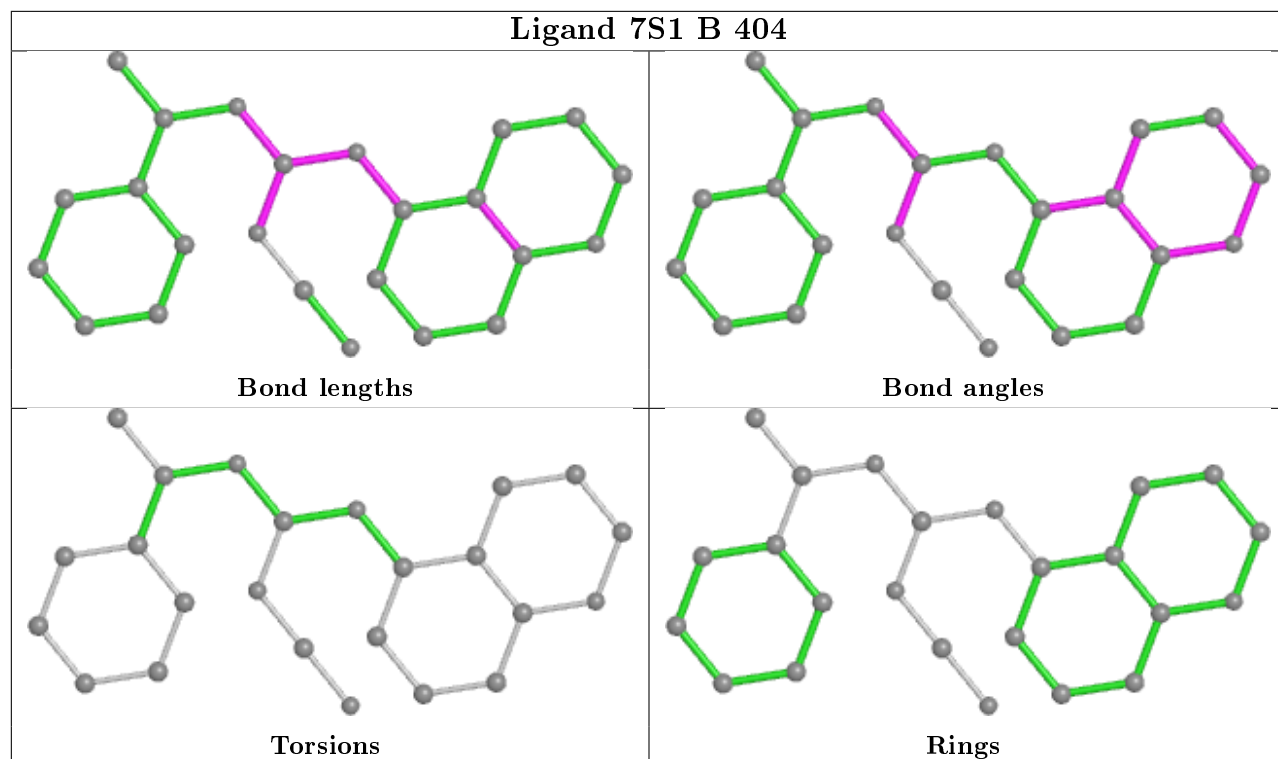
There are no ring outliers.

3 monomers are involved in 3 short contacts:

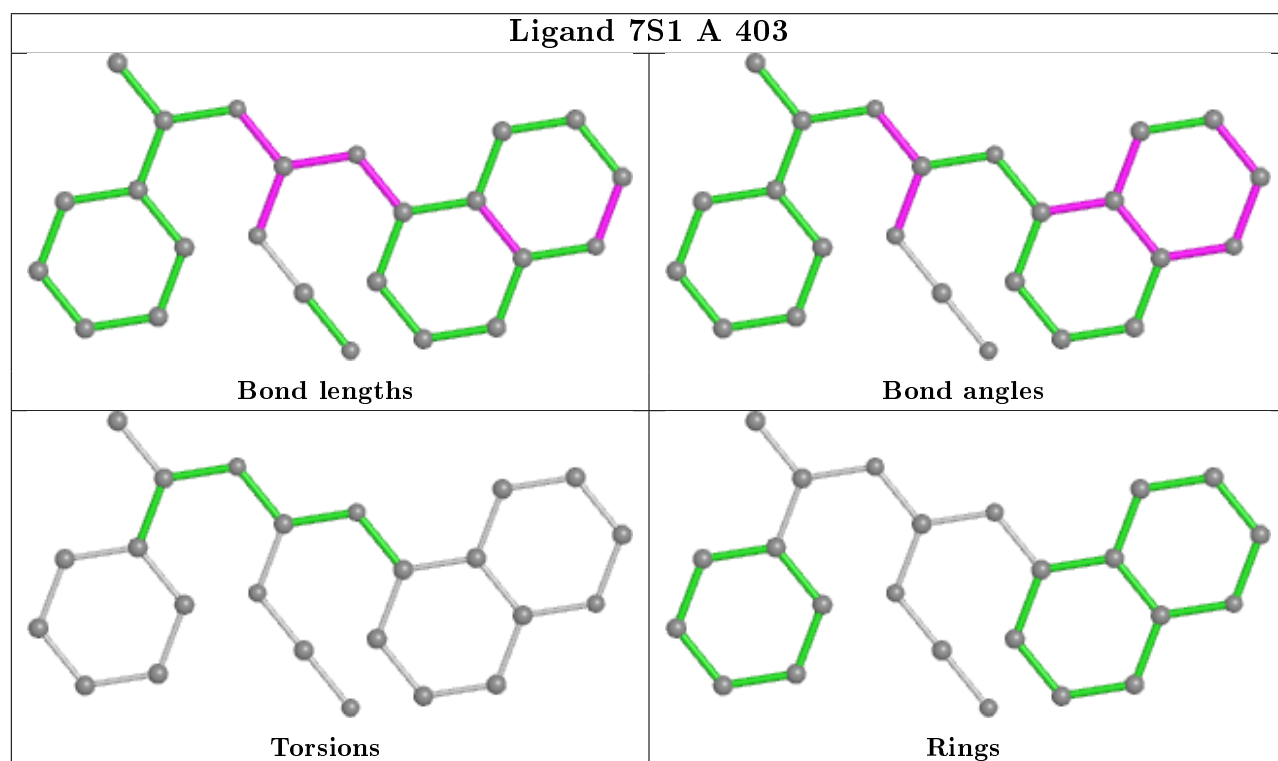
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	7S1	1	0
3	A	403	7S1	1	0
5	B	405	ATP	1	0

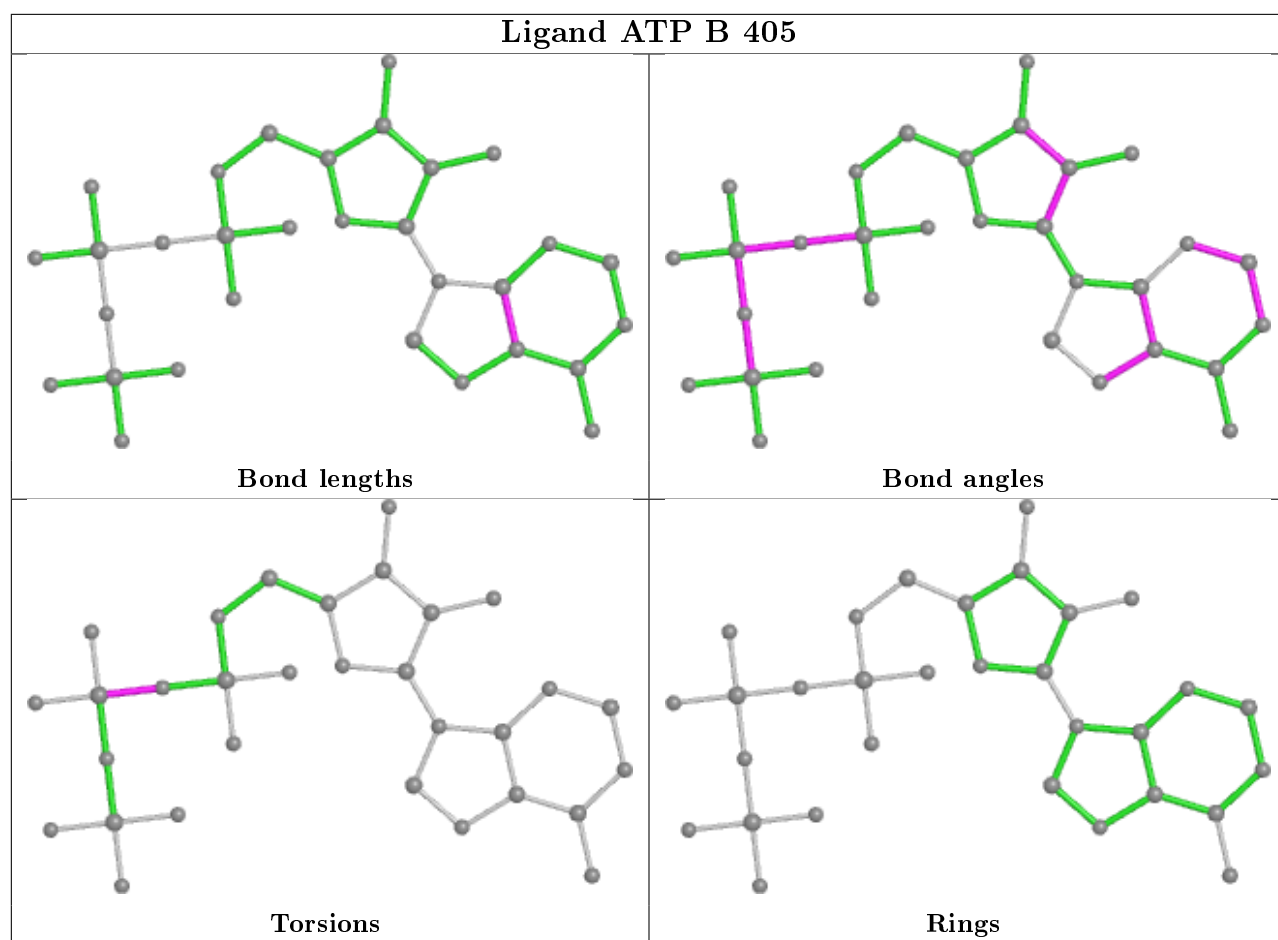
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 7S1 B 404



Ligand 7S1 A 403





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	307/342 (89%)	-0.11	19 (6%) 20 15	104, 143, 207, 221	0
1	B	299/342 (87%)	-0.05	11 (3%) 41 32	106, 144, 215, 226	0
All	All	606/684 (88%)	-0.08	30 (4%) 28 24	104, 144, 213, 226	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ASN	4.7
1	A	265	TRP	4.3
1	A	263	ASP	4.2
1	A	267	HIS	3.9
1	B	324	THR	3.5
1	A	341	ILE	3.5
1	A	266	PHE	3.2
1	A	259	ASP	3.2
1	A	264	GLY	3.2
1	A	346	LEU	3.1
1	B	259	ASP	3.0
1	A	326	GLY	3.0
1	B	216	CYS	2.8
1	A	342	SER	2.8
1	A	347	ALA	2.8
1	B	212	VAL	2.8
1	A	268	HIS	2.7
1	B	267	HIS	2.6
1	A	57	LEU	2.6
1	B	213	ASN	2.6
1	A	325	GLY	2.5
1	B	47	SER	2.4
1	A	323	GLY	2.4
1	A	345	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	348	THR	2.3
1	B	211	GLY	2.2
1	B	208	ILE	2.2
1	B	36	LEU	2.1
1	A	343	TYR	2.1
1	B	40	TYR	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](#)

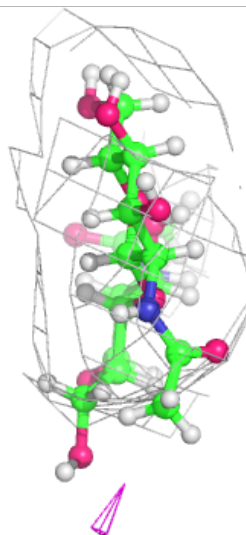
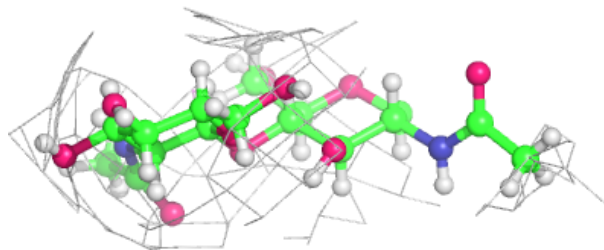
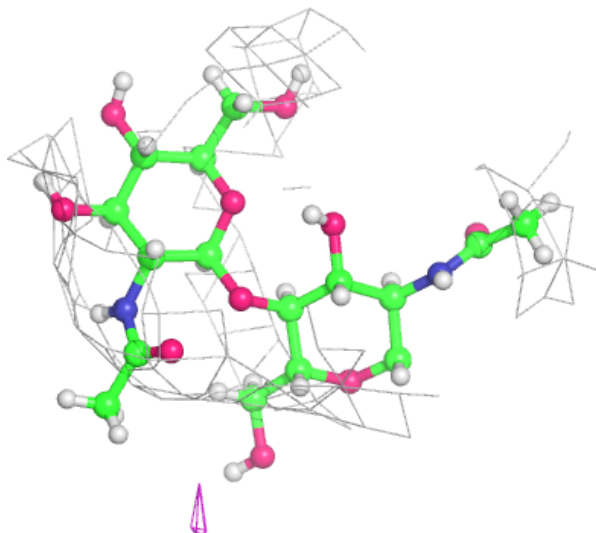
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

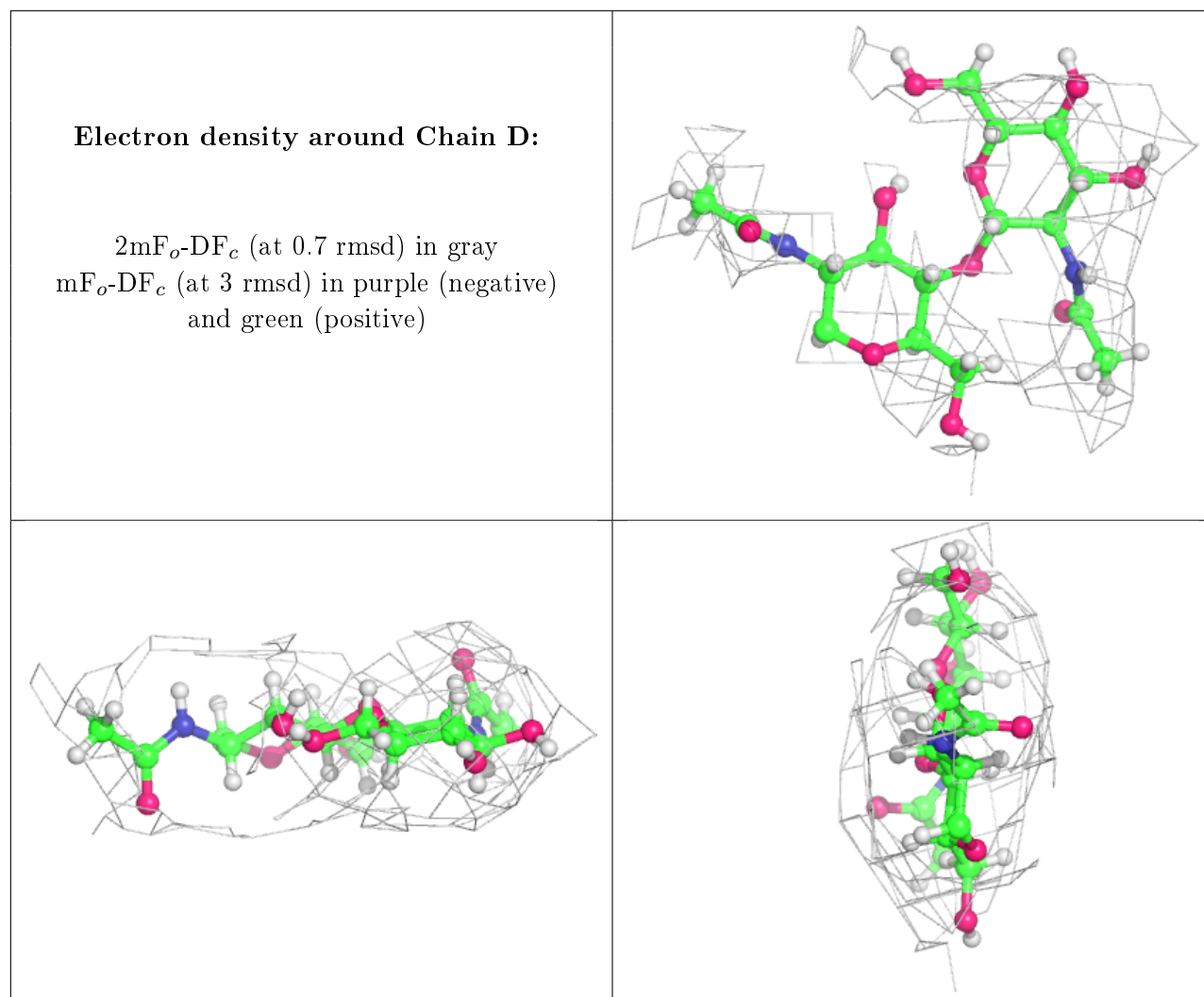
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	1	14/15	0.77	0.21	151,179,215,216	0
2	NAG	C	2	14/15	0.81	0.26	171,202,229,242	0
2	NAG	D	1	14/15	0.86	0.18	154,177,212,213	0
2	NAG	D	2	14/15	0.88	0.28	154,184,219,224	0

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

Electron density around Chain C:

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





6.4 Ligands ⓘ

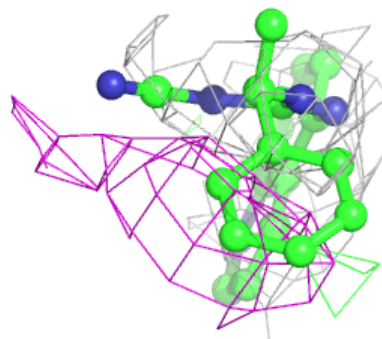
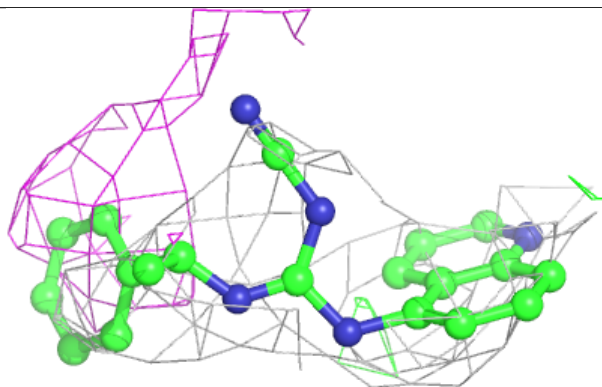
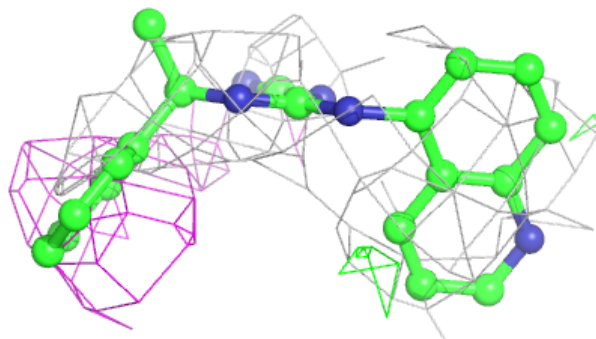
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	403	14/15	0.72	0.27	205,220,257,264	0
3	7S1	A	403	24/24	0.77	0.46	110,120,152,159	0
5	ATP	B	405	31/31	0.81	0.36	114,134,148,151	0
3	7S1	B	404	24/24	0.88	0.37	107,117,139,145	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.

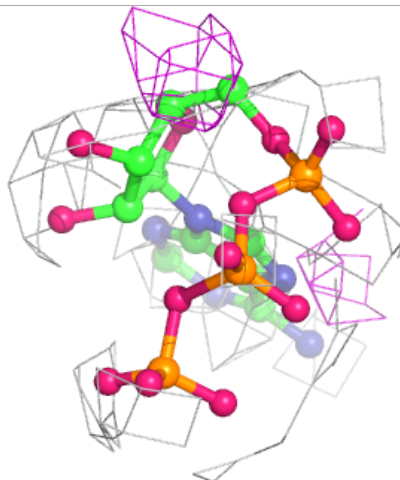
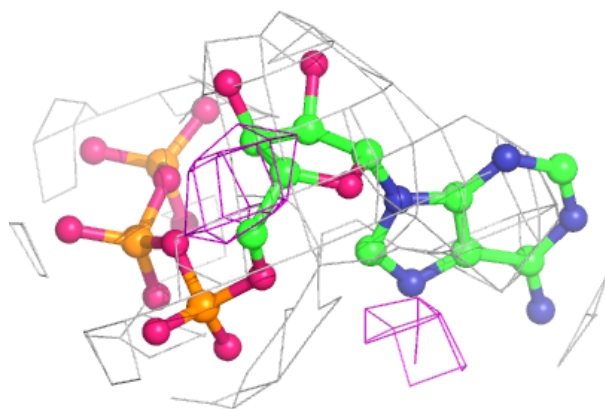
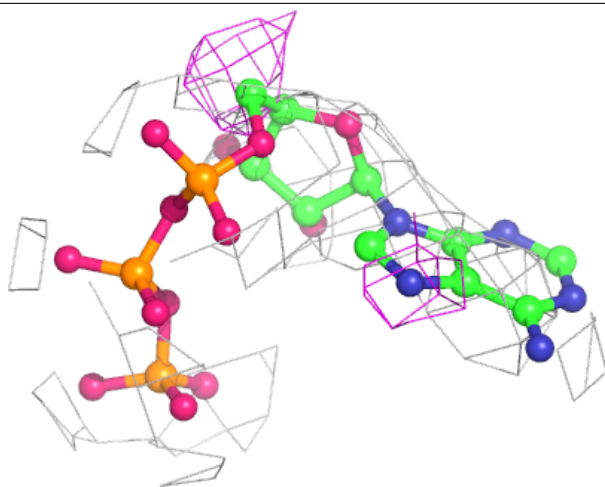
Electron density around 7S1 A 403:

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



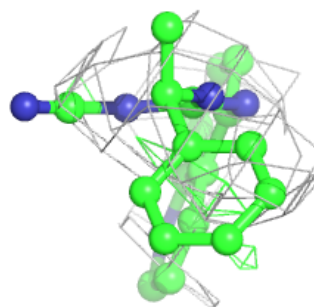
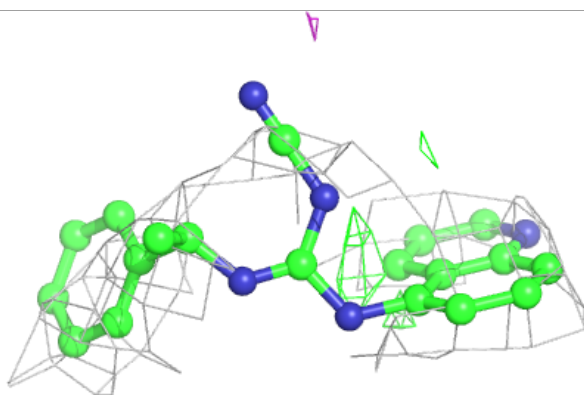
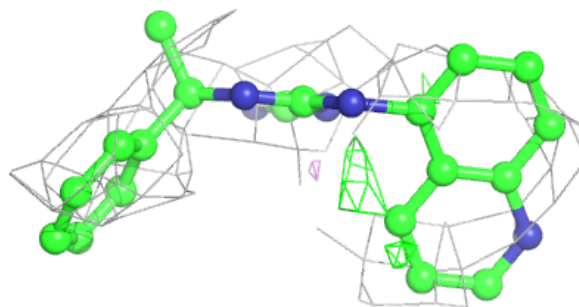
Electron density around ATP B 405:

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



Electron density around 7S1 B 404:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.