



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:56 PM UTC

PDB ID : 5U2H / pdb_00005u2h
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 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

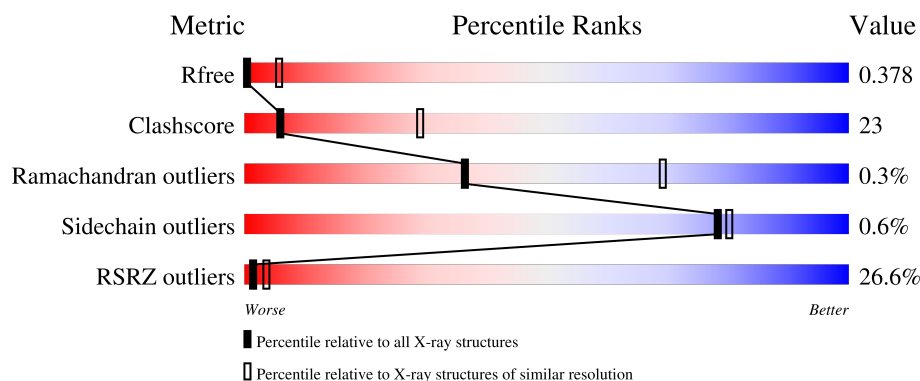
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	342	21% 61% 29% 10%
1	B	342	26% 59% 28% 13%
2	C	2	50% 50%
2	D	2	100%

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:

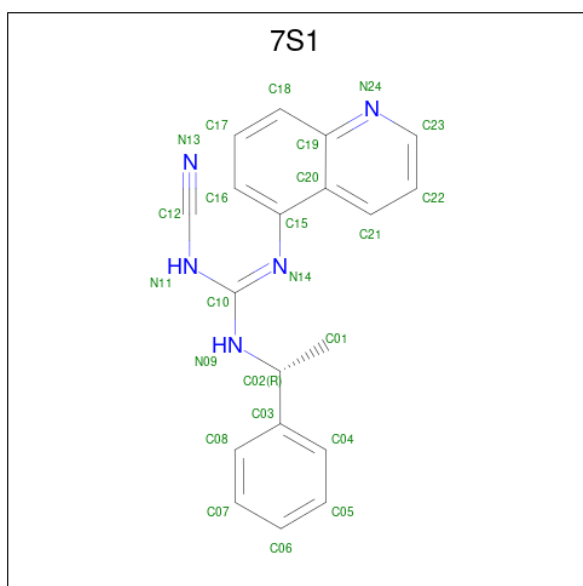
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP G1M6C4
A	22	SER	-	expression tag	UNP G1M6C4
A	35	ALA	VAL	engineered mutation	UNP G1M6C4
A	125	ALA	ARG	engineered mutation	UNP G1M6C4
A	174	LYS	GLU	engineered mutation	UNP G1M6C4
A	241	SER	ASN	engineered mutation	UNP G1M6C4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



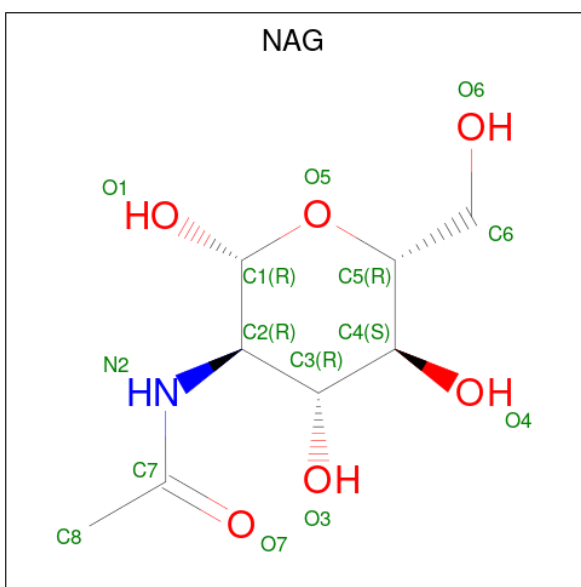
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



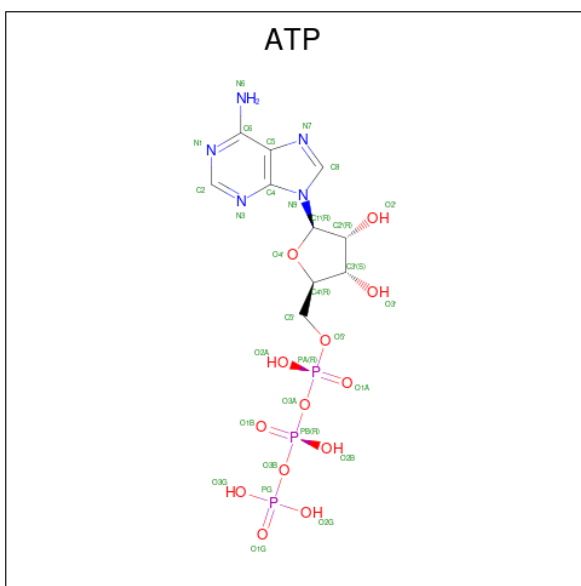
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C N	0	0
			24	19 5		
3	B	1	Total	C N	0	0
			24	19 5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

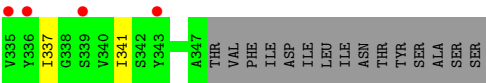


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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		



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 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) 99.9 (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 0.330 , 0.378	Depositor DCC
R_{free} test set	1446 reflections (9.94%)	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)	0.21 , 52.8	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	0.85	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: NAG, 7S1, 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	0.07	0/2062	0.23	0/2832
1	B	0.07	0/1980	0.24	0/2720
All	All	0.07	0/4042	0.23	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	88	0
1	B	1945	0	1524	76	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	167	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 23.

All (167) 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:A:234:ILE:CG2	1:A:252:MET:HE2	2.32	0.60
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
1:A:105:MET:HE2	1:A:312:VAL:HG13	1.83	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:69:ALA:HB2	1:B:188:PHE:CZ	2.39	0.56
1:B:124:THR:O	1:B:128:ILE:HG12	2.04	0.56
1:A:124:THR:HG22	1:A:125:ALA:H	1.68	0.56
1:A:234:ILE:HG21	1:A:252:MET:HE2	1.86	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:OE1	1:A:157:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C02	3:B:404:7S1:C12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:71:VAL:O	1:A:85:SER:HA	2.17	0.44
1:A:176:ALA:HB3	1:A:247:ILE:HG22	1.98	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:HA	1:B:157:GLU:OE1	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:230:ARG:HB3	1:A:233:ASP:CG	2.43	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:B:255:GLU:HG3	1:B:274:SER:HG	1.85	0.42
1:A:235:PHE:HZ	1:A:315:ILE:HD13	1.85	0.41
1:A:251:ILE:HD11	1:A:291:TYR:HD1	1.85	0.41
1:B:103:PHE:CE1	1:B:314:GLY:HA3	2.55	0.41
1:A:97:LEU:HD12	1:A:101:SER:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	69
1	B	293/342 (86%)	278 (95%)	14 (5%)	1 (0%)	36	69
All	All	594/684 (87%)	568 (96%)	24 (4%)	2 (0%)	36	69

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%)	78	80
1	B	151/300 (50%)	150 (99%)	1 (1%)	76	78
All	All	311/600 (52%)	309 (99%)	2 (1%)	78	80

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

Mol	Chain	Res	Type
1	A	182	LEU
1	B	152	CYS

Sometimes 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	2,1	14,14,15	0.23	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.17	0	17,19,21	0.44	0
2	NAG	D	1	2,1	14,14,15	0.29	0	17,19,21	0.54	0
2	NAG	D	2	2	14,14,15	0.19	0	17,19,21	0.42	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
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.

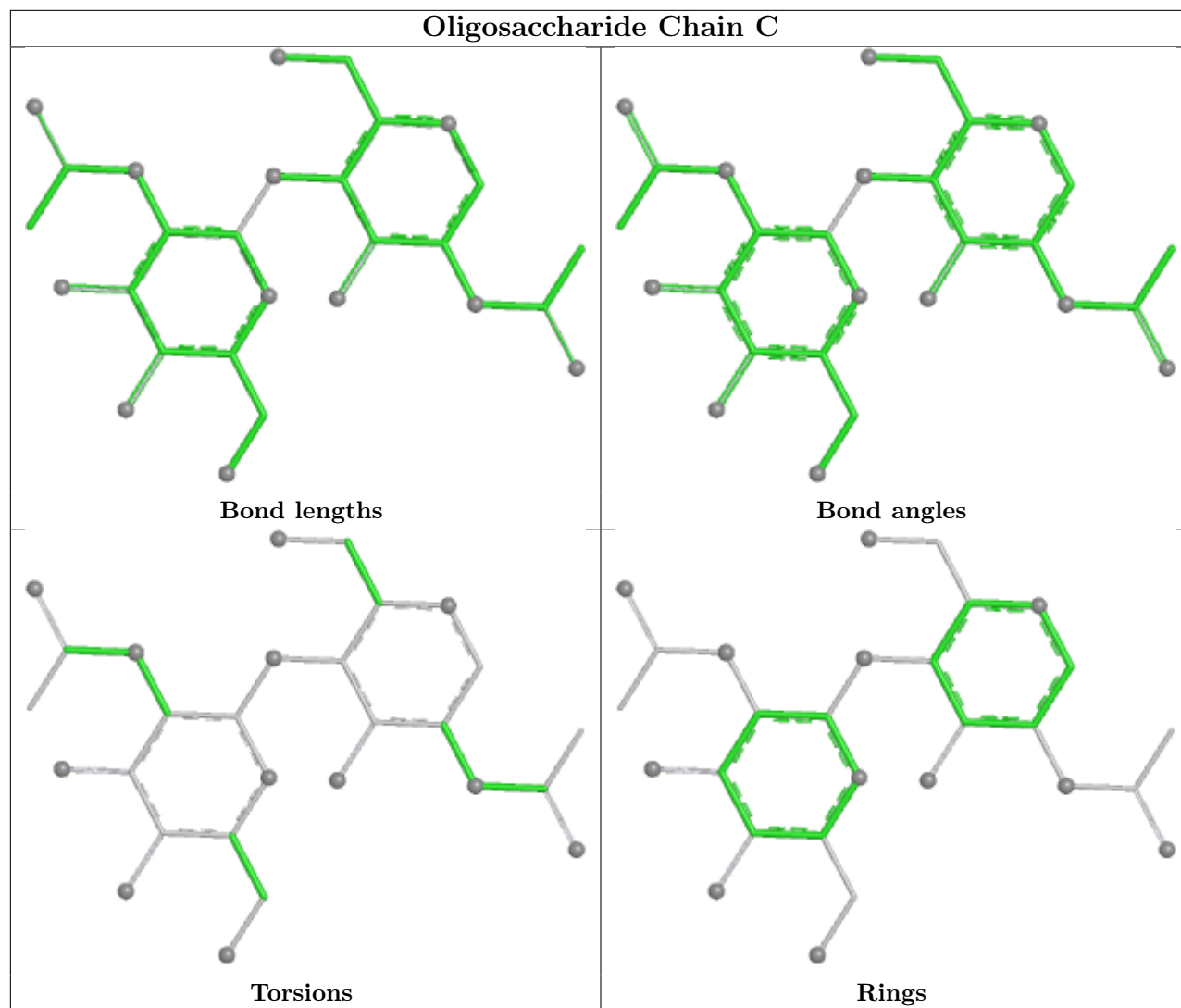
There are no torsion outliers.

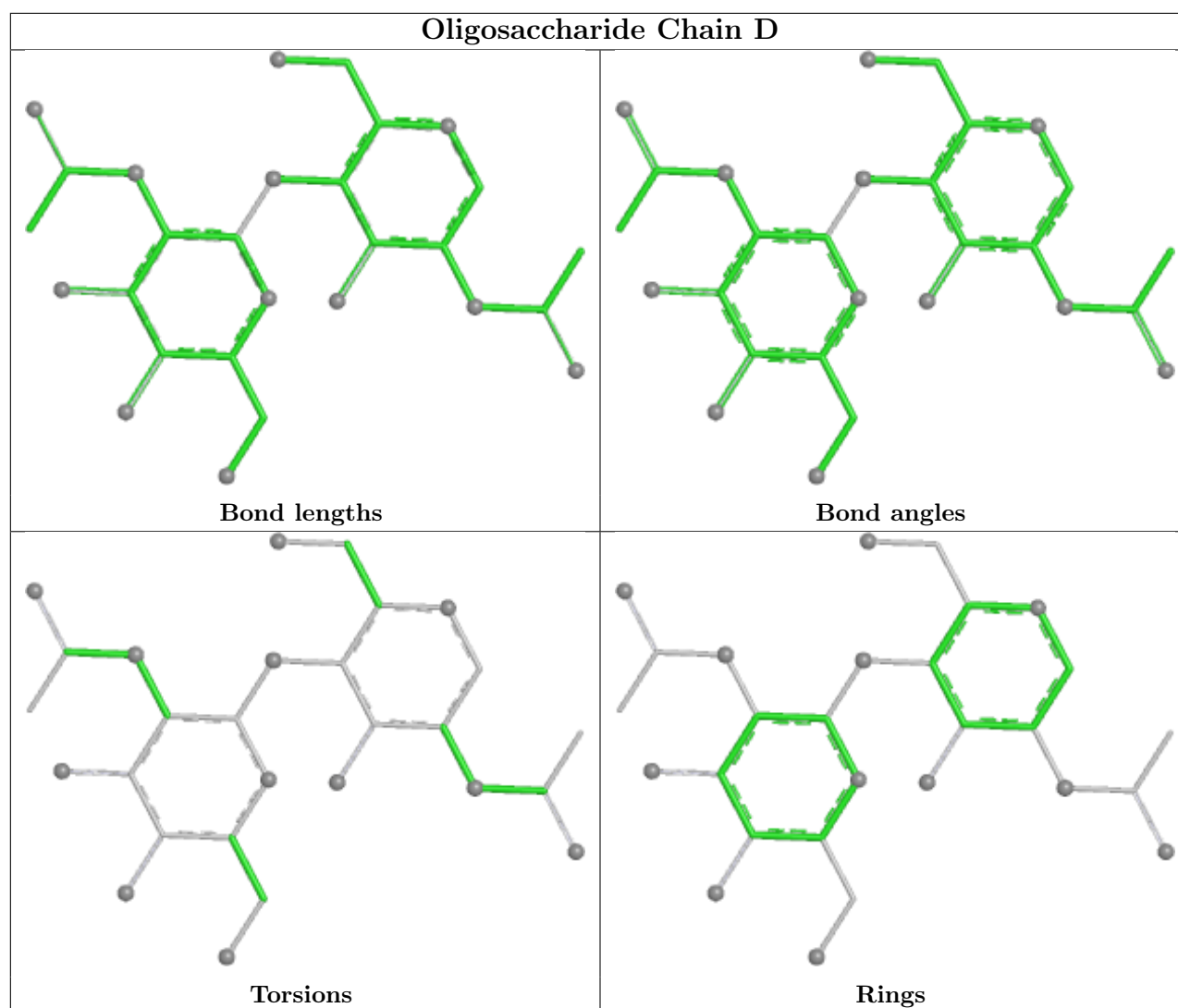
There are no ring outliers.

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	$\# Z > 2$
4	NAG	B	403	1	14,14,15	0.21	0	17,19,21	0.47	0
3	7S1	B	404	-	25,26,26	2.74	6 (24%)	30,34,34	1.33	4 (13%)
3	7S1	A	403	-	25,26,26	2.72	6 (24%)	30,34,34	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	B	405	-	32,33,33	1.39	4 (12%)	48,52,52	1.77	8 (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
4	NAG	B	403	1	-	1/6/23/26	0/1/1/1
3	7S1	B	404	-	-	2/12/15/15	0/3/3/3
3	7S1	A	403	-	-	1/12/15/15	0/3/3/3
5	ATP	B	405	-	-	1/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	7S1	C10-N11	8.01	1.48	1.38
3	A	403	7S1	C10-N11	7.86	1.48	1.38
3	A	403	7S1	C10-N14	7.19	1.49	1.30
3	B	404	7S1	C10-N14	7.15	1.49	1.30
3	B	404	7S1	C15-N14	4.99	1.49	1.41
3	A	403	7S1	C15-N14	4.91	1.49	1.41
5	B	405	ATP	C5-C4	4.72	1.47	1.39
3	B	404	7S1	C20-C19	-3.37	1.37	1.42
3	A	403	7S1	C20-C19	-3.34	1.37	1.42
3	B	404	7S1	C10-N09	-3.06	1.29	1.35
3	A	403	7S1	C10-N09	-3.01	1.29	1.35
5	B	405	ATP	C5-C6	2.73	1.48	1.41
5	B	405	ATP	C8-N7	2.31	1.36	1.31
5	B	405	ATP	C5-N7	-2.27	1.34	1.39
3	A	403	7S1	C23-N24	2.11	1.36	1.32
3	B	404	7S1	C23-N24	2.05	1.36	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	405	ATP	C5-C4-N3	-5.87	118.64	126.72
5	B	405	ATP	N3-C4-N9	4.67	135.11	127.17
3	A	403	7S1	N09-C10-N11	3.91	125.68	116.80
3	B	404	7S1	N09-C10-N11	3.90	125.64	116.80
5	B	405	ATP	C2-N3-C4	3.67	120.80	111.83
5	B	405	ATP	C4-C5-N7	-3.41	106.68	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	405	ATP	N3-C2-N1	-3.18	123.76	128.58
3	A	403	7S1	C21-C20-C15	-2.67	120.03	123.25
3	B	404	7S1	C21-C20-C15	-2.63	120.08	123.25
3	A	403	7S1	C22-C23-N24	-2.63	120.11	123.97
5	B	405	ATP	C4-N9-C8	2.61	108.48	105.74
3	B	404	7S1	C22-C23-N24	-2.53	120.25	123.97
5	B	405	ATP	C5-N7-C8	2.50	107.38	103.45
3	A	403	7S1	C20-C19-N24	-2.38	120.30	122.82
3	B	404	7S1	C20-C19-N24	-2.35	120.33	122.82
5	B	405	ATP	C3'-C2'-C1'	2.29	105.80	101.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	NAG	C1-C2-N2-C7
5	B	405	ATP	PA-O3A-PB-O1B
3	A	403	7S1	C01-C02-N09-C10
3	B	404	7S1	C01-C02-N09-C10
3	B	404	7S1	C03-C02-N09-C10

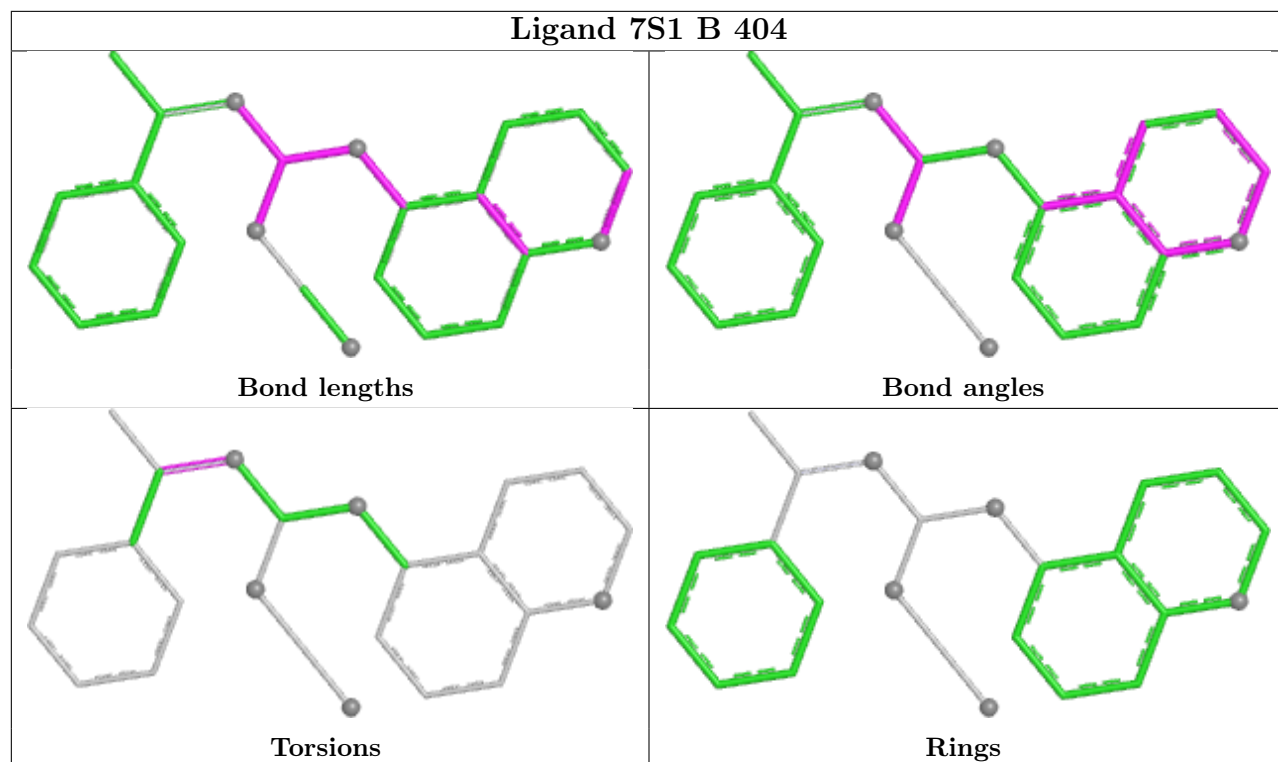
There are no ring outliers.

3 monomers are involved in 3 short contacts:

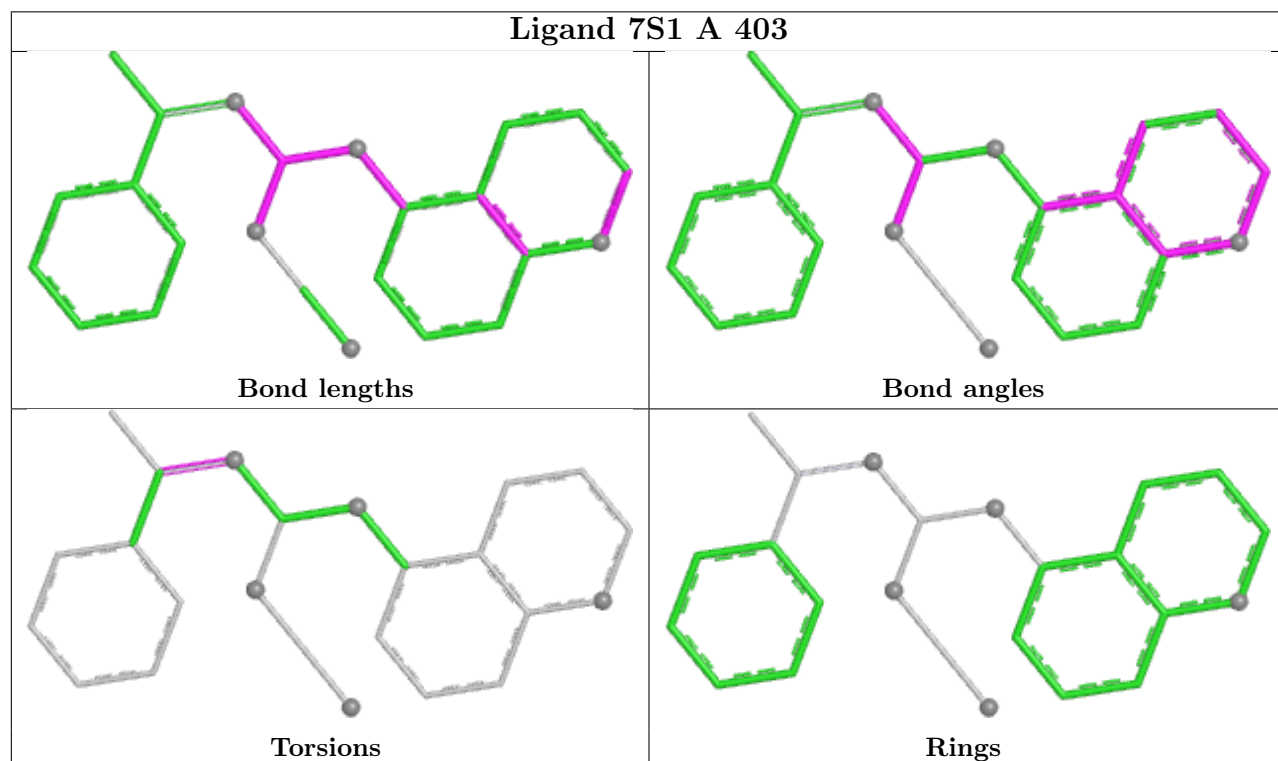
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	7S1	1	0
3	A	403	7S1	1	0
5	B	405	ATP	1	0

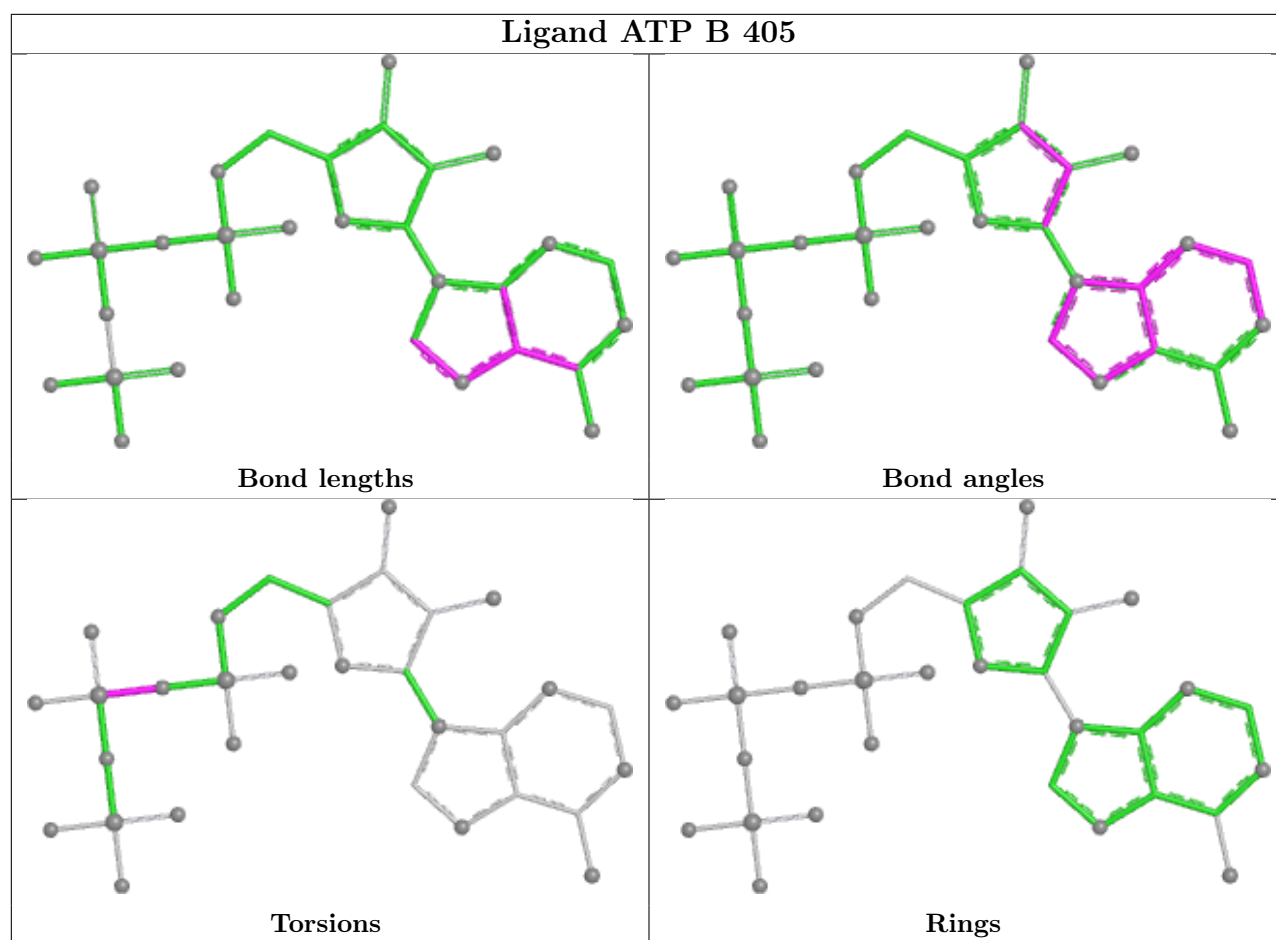
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	1.37	72 (23%) 2 4	104, 143, 207, 221	0
1	B	299/342 (87%)	1.62	89 (29%) 1 3	106, 144, 215, 226	0
All	All	606/684 (88%)	1.50	161 (26%) 1 3	104, 144, 212, 226	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLN	8.9
1	A	79	GLY	7.6
1	B	213	ASN	7.1
1	B	208	ILE	7.1
1	B	99	GLY	7.0
1	B	323	GLY	6.6
1	B	100	ASN	6.1
1	A	295	TYR	5.9
1	B	288	TYR	5.6
1	B	63	THR	5.5
1	B	216	CYS	5.3
1	A	288	TYR	5.3
1	A	177	PRO	5.2
1	B	97	LEU	5.1
1	A	341	ILE	5.1
1	B	95	PHE	4.6
1	B	196	ILE	4.6
1	B	295	TYR	4.6
1	A	95	PHE	4.6
1	B	286	SER	4.5
1	A	142	PRO	4.5
1	A	326	GLY	4.4
1	B	269	CYS	4.4
1	B	259	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	252	MET	4.0
1	A	325	GLY	4.0
1	B	79	GLY	3.9
1	A	227	PRO	3.9
1	A	57	LEU	3.9
1	B	276	ARG	3.9
1	A	62	HIS	3.8
1	B	214	ILE	3.8
1	B	263	ASP	3.8
1	A	201	HIS	3.8
1	B	125	ALA	3.7
1	A	98	GLN	3.7
1	A	99	GLY	3.7
1	A	263	ASP	3.7
1	A	283	THR	3.6
1	B	209	LEU	3.5
1	B	201	HIS	3.5
1	B	56	PRO	3.5
1	B	212	VAL	3.5
1	B	65	VAL	3.4
1	A	174	LYS	3.4
1	A	228	ILE	3.4
1	A	296	ALA	3.4
1	A	265	TRP	3.4
1	A	205	THR	3.3
1	A	259	ASP	3.3
1	B	101	SER	3.3
1	B	102	PHE	3.3
1	B	211	GLY	3.3
1	B	324	THR	3.3
1	A	206	ARG	3.3
1	B	80	MET	3.3
1	A	267	HIS	3.3
1	A	75	ILE	3.2
1	B	96	PRO	3.2
1	A	141	ASP	3.1
1	A	65	VAL	3.1
1	A	291	TYR	3.1
1	A	343	TYR	3.1
1	B	207	ASN	3.1
1	B	192	ILE	3.0
1	A	294	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	48	ASP	3.0
1	A	63	THR	3.0
1	B	215	THR	3.0
1	B	36	LEU	3.0
1	B	339	SER	3.0
1	B	143	GLN	2.9
1	B	182	LEU	2.9
1	A	346	LEU	2.9
1	B	175	ASP	2.8
1	B	321	VAL	2.8
1	A	158	ARG	2.8
1	A	191	LEU	2.8
1	B	205	THR	2.8
1	A	261	ASN	2.8
1	A	342	SER	2.8
1	A	189	THR	2.8
1	A	164	VAL	2.7
1	A	94	THR	2.7
1	B	279	ASP	2.7
1	B	210	PRO	2.7
1	B	260	CYS	2.7
1	A	56	PRO	2.7
1	B	124	THR	2.7
1	A	52	GLN	2.6
1	A	215	THR	2.6
1	A	214	ILE	2.6
1	B	289	PRO	2.6
1	B	189	THR	2.6
1	B	61	VAL	2.6
1	B	190	VAL	2.6
1	B	40	TYR	2.6
1	B	238	THR	2.6
1	B	299	TYR	2.6
1	B	171	GLU	2.6
1	A	199	PRO	2.6
1	A	46	ILE	2.6
1	B	77	GLU	2.6
1	A	200	GLY	2.6
1	B	228	ILE	2.5
1	B	206	ARG	2.5
1	B	280	ASP	2.5
1	B	335	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	142	PRO	2.5
1	A	268	HIS	2.5
1	B	194	ASN	2.5
1	B	291	TYR	2.5
1	A	176	ALA	2.4
1	A	59	SER	2.4
1	A	53	LYS	2.4
1	B	336	TYR	2.4
1	A	78	ASN	2.4
1	A	171	GLU	2.4
1	B	73	ALA	2.4
1	B	275	PHE	2.4
1	B	37	VAL	2.4
1	B	154	VAL	2.3
1	B	294	ARG	2.3
1	A	54	LYS	2.3
1	B	64	LYS	2.3
1	B	71	VAL	2.3
1	B	251	ILE	2.3
1	B	45	LEU	2.3
1	B	128	ILE	2.3
1	A	148	GLN	2.3
1	A	197	ASP	2.3
1	A	96	PRO	2.2
1	A	344	PHE	2.2
1	B	179	PRO	2.2
1	B	278	LEU	2.2
1	A	345	GLY	2.2
1	B	267	HIS	2.2
1	B	158	ARG	2.2
1	A	190	VAL	2.2
1	A	289	PRO	2.2
1	B	318	ASP	2.1
1	A	192	ILE	2.1
1	B	258	TRP	2.1
1	A	323	GLY	2.1
1	A	248	GLN	2.1
1	A	50	ARG	2.1
1	A	203	TYR	2.1
1	B	264	GLY	2.1
1	A	110	LYS	2.1
1	B	72	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.1
1	A	280	ASP	2.0
1	A	34	HIS	2.0
1	B	120	PRO	2.0
1	B	170	ILE	2.0
1	A	340	VAL	2.0
1	A	269	CYS	2.0
1	B	138	GLY	2.0
1	B	343	TYR	2.0
1	B	39	SER	2.0
1	B	180	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

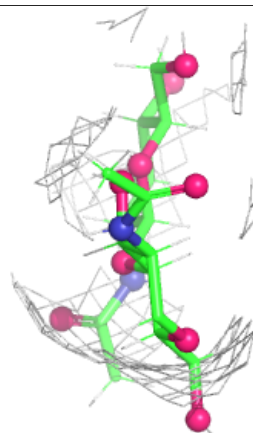
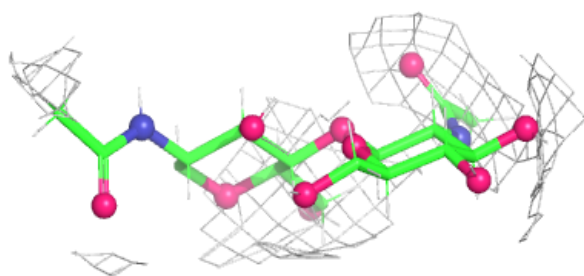
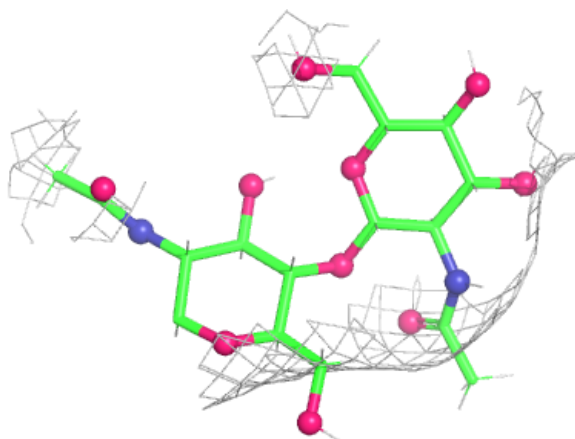
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

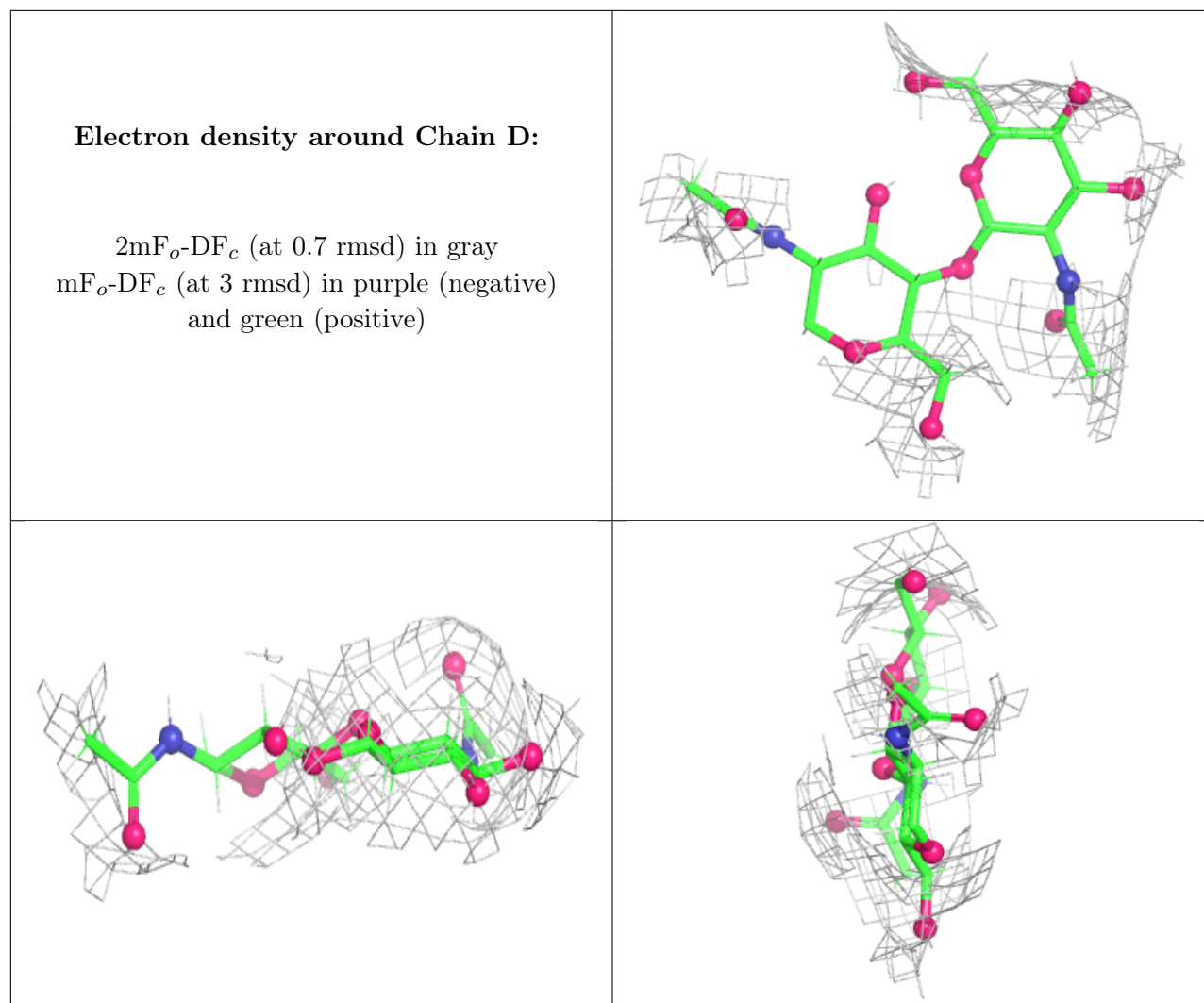
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.45	0.11	154,184,219,224	0
2	NAG	C	1	14/15	0.52	0.16	151,179,215,216	0
2	NAG	D	1	14/15	0.57	0.12	154,177,212,213	0
2	NAG	C	2	14/15	0.68	0.14	171,202,229,242	0

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 [i](#)

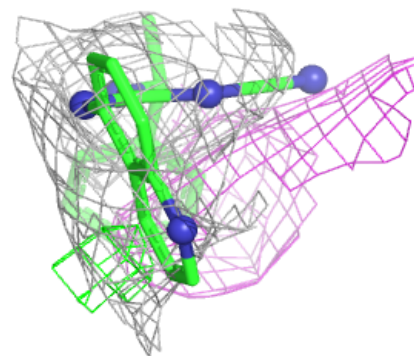
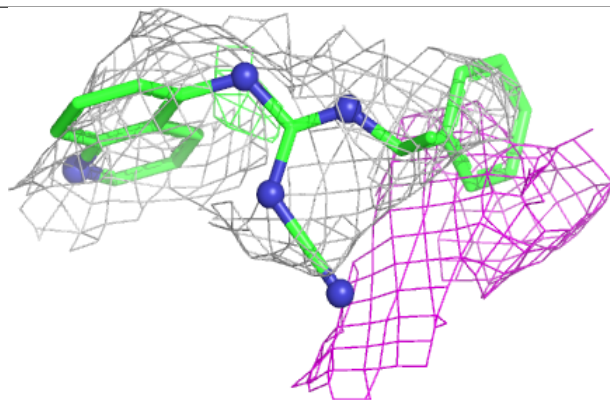
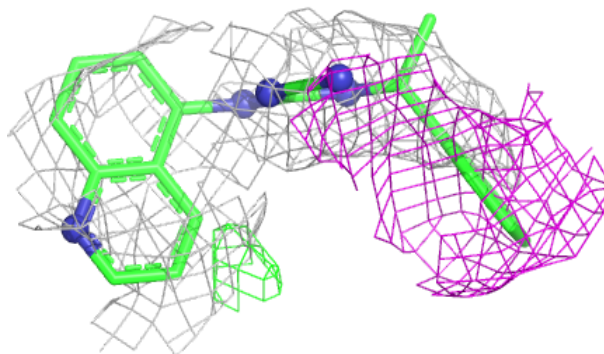
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	403	14/15	0.50	0.13	205,220,257,264	0
3	7S1	A	403	24/24	0.80	0.35	110,120,152,159	0
5	ATP	B	405	31/31	0.89	0.14	114,134,148,151	0
3	7S1	B	404	24/24	0.92	0.26	107,117,139,145	0

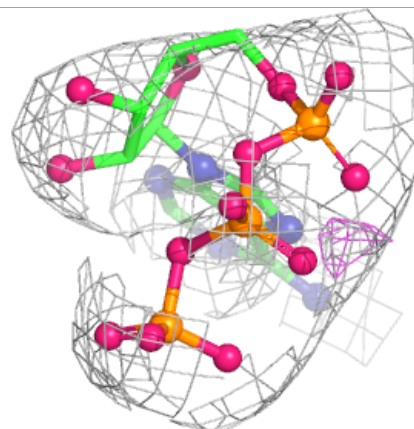
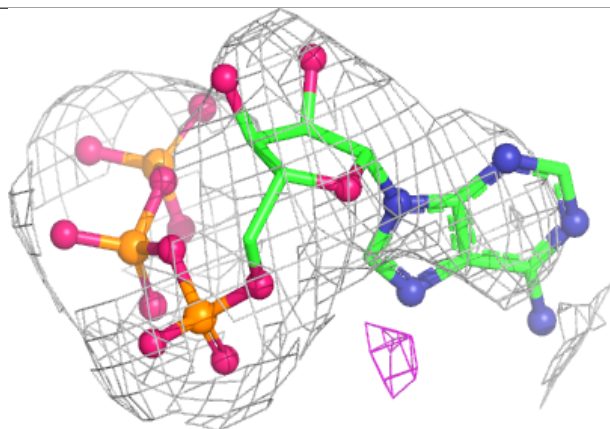
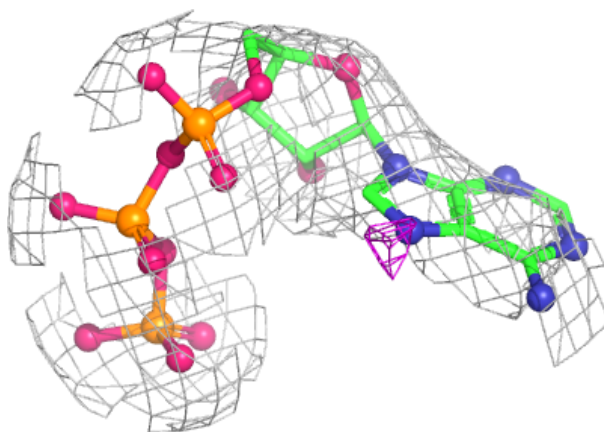
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

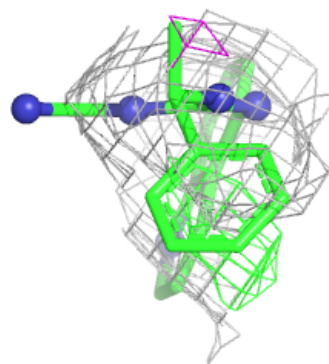
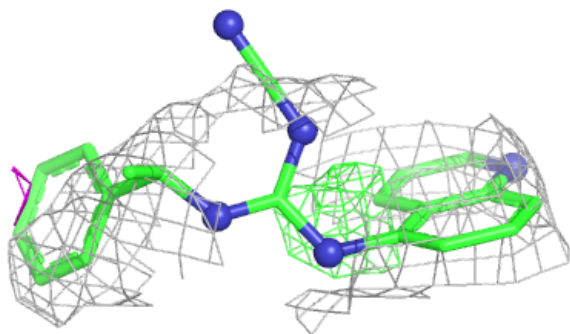
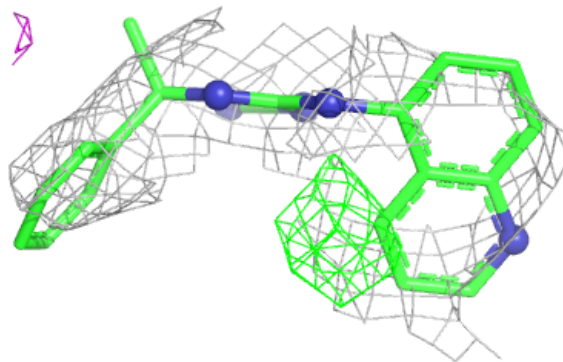
**Electron density around ATP B 405:**

$2mF_o-DF_c$ (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.