



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2025 – 03:39 pm GMT

PDB ID : 9R0H / pdb_00009r0h
Title : Human CD73 (ecto 5'-nucleotidase) in complex with compound 6 (ORIC-533)
Authors : Moore, J.T.; Ivic, N.; Lammens, A.; Krapp, S.; Maskos, K.
Deposited on : 2025-04-24
Resolution : 2.28 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

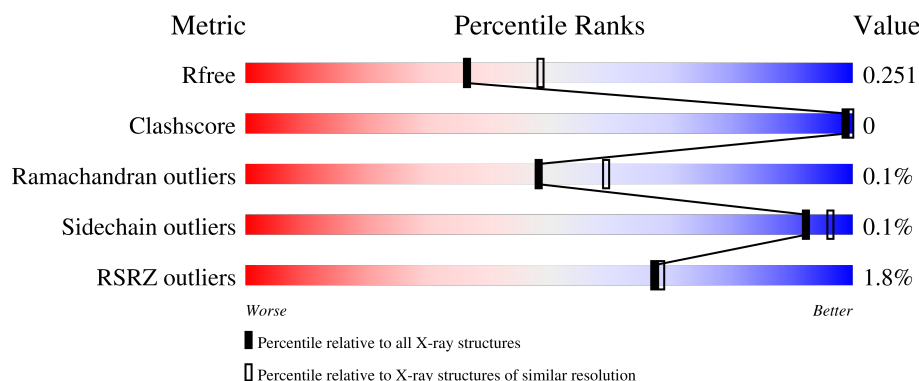
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

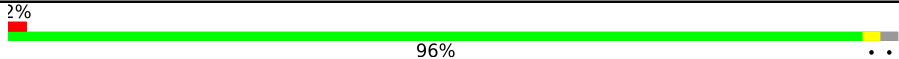
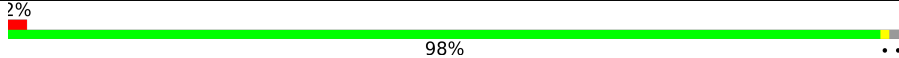
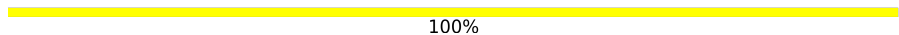
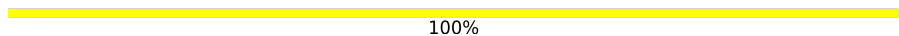
The reported resolution of this entry is 2.28 Å.

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	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	533	 2% 96%
1	B	533	 2% 98%
2	C	2	 100%
2	D	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8869 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	61	5	0
			4135	2628	705	782	20			
1	B	525	Total	C	N	O	S	55	3	0
			4120	2617	705	778	20			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP P21589
A	24	ALA	-	expression tag	UNP P21589
A	25	SER	-	expression tag	UNP P21589
A	26	MET	-	expression tag	UNP P21589
A	53	ASP	ASN	engineered mutation	UNP P21589
A	333	ASP	ASN	engineered mutation	UNP P21589
A	403	ASP	ASN	engineered mutation	UNP P21589
A	550	HIS	-	expression tag	UNP P21589
A	551	HIS	-	expression tag	UNP P21589
A	552	HIS	-	expression tag	UNP P21589
A	553	HIS	-	expression tag	UNP P21589
A	554	HIS	-	expression tag	UNP P21589
A	555	HIS	-	expression tag	UNP P21589
B	23	LEU	-	expression tag	UNP P21589
B	24	ALA	-	expression tag	UNP P21589
B	25	SER	-	expression tag	UNP P21589
B	26	MET	-	expression tag	UNP P21589
B	53	ASP	ASN	engineered mutation	UNP P21589
B	333	ASP	ASN	engineered mutation	UNP P21589
B	403	ASP	ASN	engineered mutation	UNP P21589
B	550	HIS	-	expression tag	UNP P21589
B	551	HIS	-	expression tag	UNP P21589
B	552	HIS	-	expression tag	UNP P21589
B	553	HIS	-	expression tag	UNP P21589
B	554	HIS	-	expression tag	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
B	555	HIS	-	expression tag	UNP P21589

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

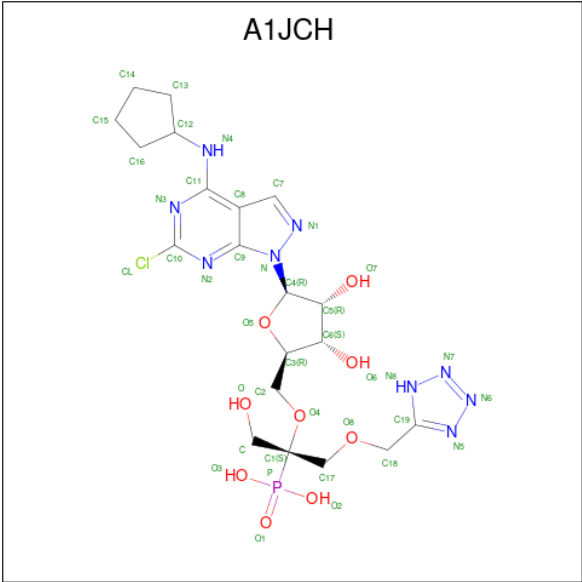
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

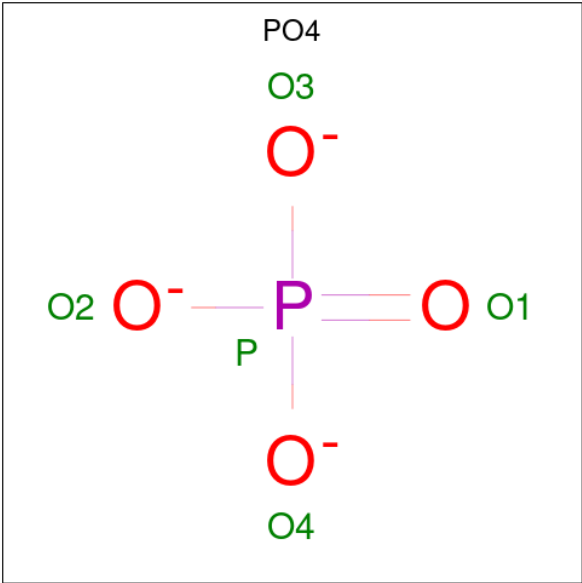
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is [(2 {S})-2-[(2 {R},3 {S},4 {R},5 {R})-5-[6-chloranyl-4-(cyclopentylamino)pyrazolo[3,4-d]pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy]-1-oxidanyl-3-(1 {H}-1,2,3,4-tetrazol-5-ylmethoxy)propan-2-yl]phosphonic acid (CCD ID: A1JCH) (formula: C₂₀H₂₉ClN₉O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	P	0	1
			48	23	1	13	10	1		
5	B	1	Total	C	Cl	N	O	P	0	1
			48	23	1	13	10	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

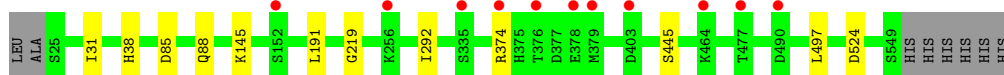


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	236	Total 236	O 236	0	0
7	B	210	Total 210	O 210	0	0

- Molecule 1: 5'-nucleotidase



- [illegible]

- NAG1
NAG2

- NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	230.96Å 93.03Å 54.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.48 – 2.28 115.48 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.6 (115.48-2.28) 98.6 (115.48-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.198 , 0.252 0.203 , 0.251	Depositor DCC
R_{free} test set	1327 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8869	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9011e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, PO4, ZN, CA, A1JCH

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	0.85	2/4221 (0.0%)	1.01	3/5713 (0.1%)
1	B	0.84	1/4207 (0.0%)	1.00	1/5694 (0.0%)
All	All	0.85	3/8428 (0.0%)	1.01	4/11407 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	ARG	NE-CZ	6.21	1.39	1.33
1	B	234	ARG	CD-NE	-5.57	1.38	1.46
1	A	191	LEU	CA-C	5.18	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	GLY	N-CA-C	6.31	120.34	111.19
1	A	145	LYS	O-C-N	6.04	130.28	123.27
1	A	219	GLY	N-CA-C	5.62	119.76	110.55
1	A	524	ASP	N-CA-C	5.13	117.27	111.11

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	4135	0	4116	3	0
1	B	4120	0	4089	4	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	48	0	0	1	0
5	B	48	0	0	3	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	236	0	0	0	0
7	B	210	0	0	1	0
All	All	8869	0	8255	7	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (7) 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:350[B]:SER:HB2	5:B:604[B]:A1JCH:N6	1.96	0.80
1:B:350[B]:SER:CB	5:B:604[B]:A1JCH:N6	2.55	0.69
1:B:49:SER:HA	7:B:836:HOH:O	2.09	0.52
1:A:445:SER:OG	5:A:604[B]:A1JCH:N7	2.42	0.52
1:B:445:SER:OG	5:B:604[B]:A1JCH:N7	2.45	0.47
1:A:38:HIS:CE1	1:A:85:ASP:HB3	2.55	0.42
1:A:31:ILE:HD12	1:A:292:ILE:HD11	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/533 (99%)	512 (97%)	15 (3%)	1 (0%)	44	53
1	B	524/533 (98%)	506 (97%)	18 (3%)	0	100	100
All	All	1052/1066 (99%)	1018 (97%)	33 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLN

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	458/460 (100%)	457 (100%)	1 (0%)	92	96
1	B	456/460 (99%)	456 (100%)	0	100	100
All	All	914/920 (99%)	913 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	190	ASN
1	A	382	ASN
1	A	526	ASN
1	B	88	GLN
1	B	252	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 ⓘ

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	0.52	0	17,19,21	1.62	2 (11%)
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	1.57	3 (17%)
2	NAG	D	1	2,1	14,14,15	0.45	0	17,19,21	1.65	2 (11%)
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	1.10	1 (5%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	1	NAG	C2-N2-C7	3.99	128.58	122.90
2	C	1	NAG	C8-C7-N2	3.60	122.20	116.10
2	C	2	NAG	C2-N2-C7	3.42	127.78	122.90
2	C	1	NAG	C2-N2-C7	3.32	127.63	122.90
2	D	1	NAG	C8-C7-N2	3.29	121.68	116.10
2	C	2	NAG	C8-C7-N2	3.10	121.35	116.10
2	D	2	NAG	C1-O5-C5	3.08	116.37	112.19
2	C	2	NAG	C1-O5-C5	2.33	115.35	112.19

There are no chirality outliers.

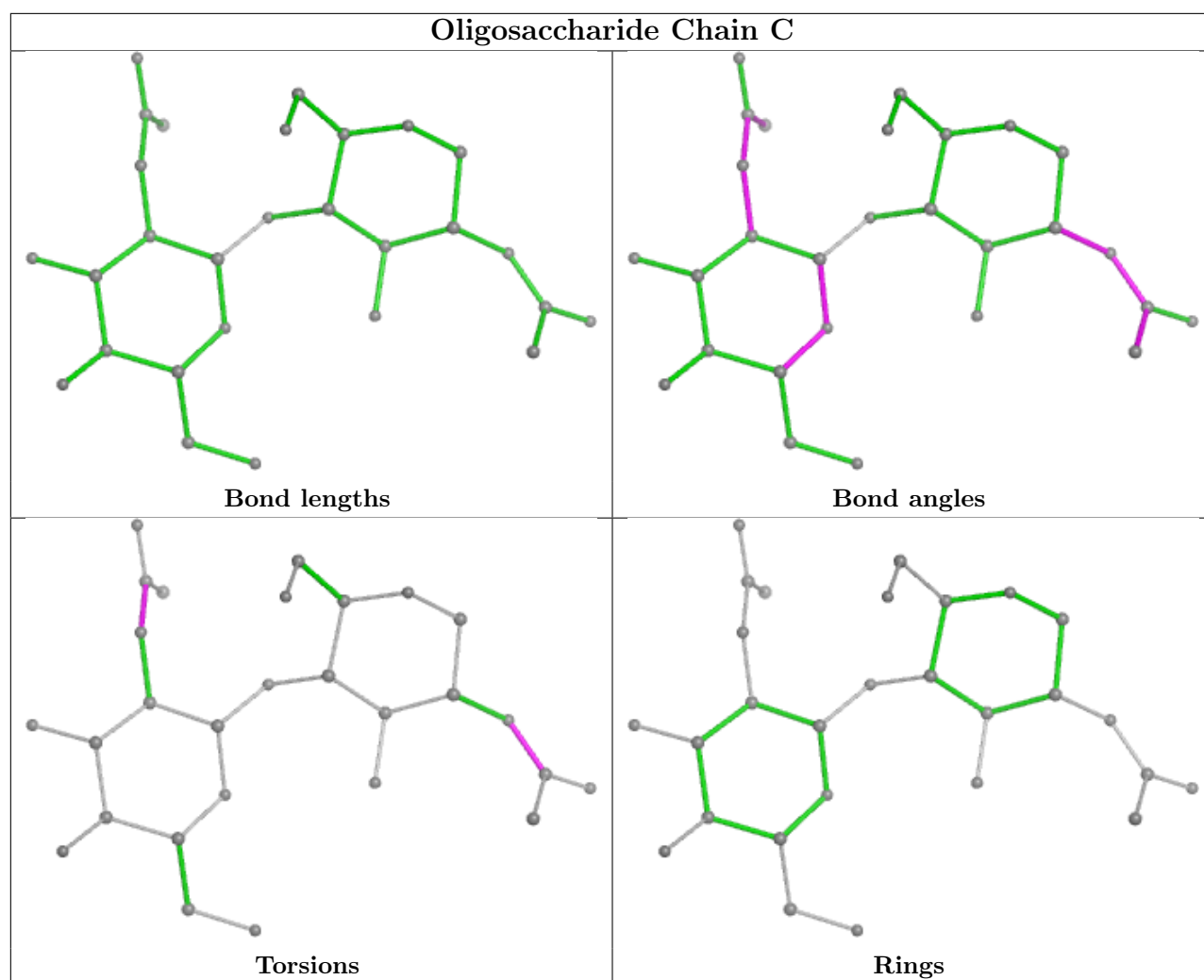
All (6) torsion outliers are listed below:

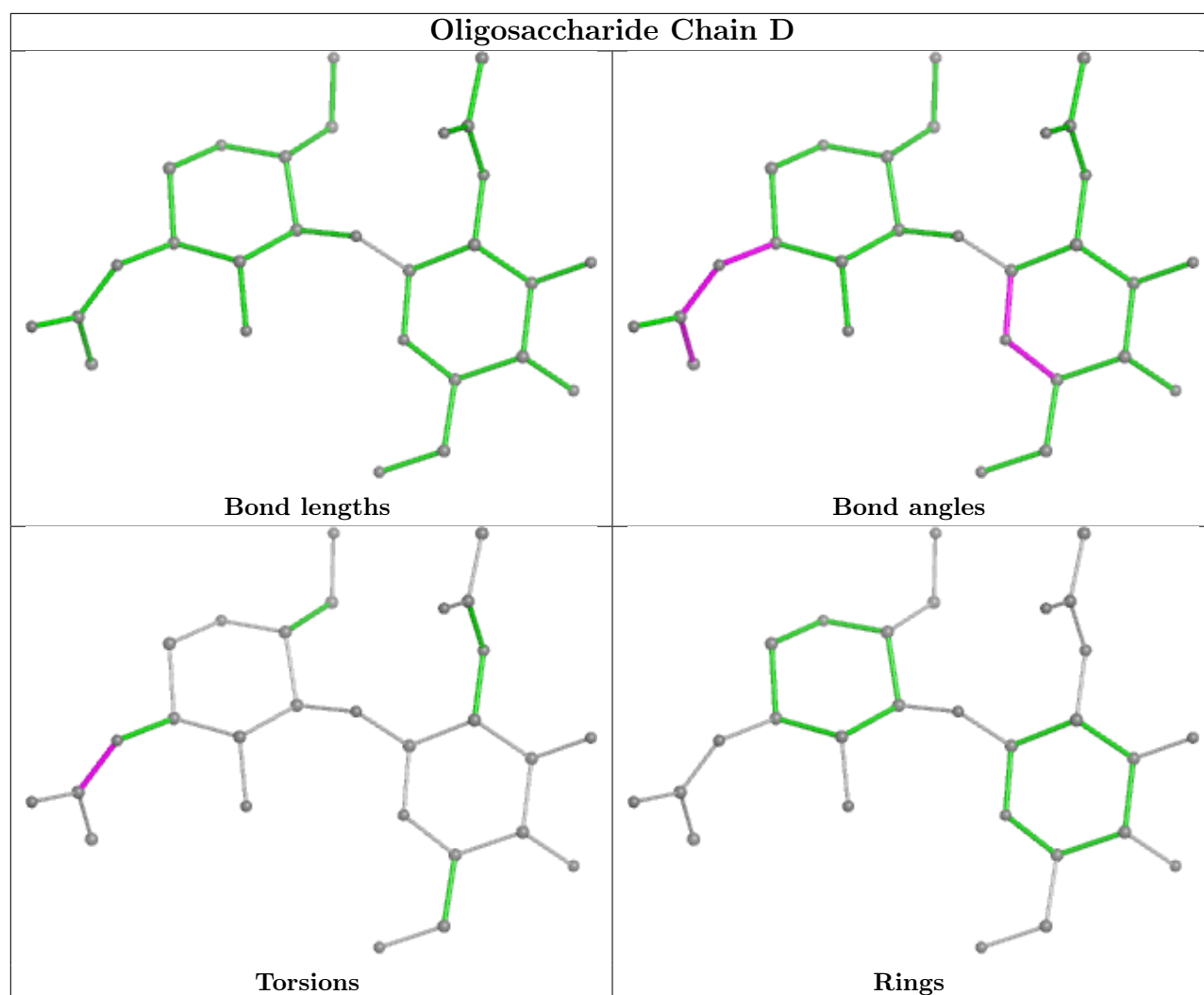
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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$
6	PO4	A	605	-	4,4,4	0.85	0	6,6,6	0.48	0
5	A1JCH	A	604[A]	-	37,44,44	0.80	1 (2%)	40,65,65	1.40	4 (10%)
5	A1JCH	A	604[B]	-	37,44,44	0.81	1 (2%)	40,65,65	1.50	5 (12%)
6	PO4	B	605	-	4,4,4	0.92	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1JCH	B	604[A]	-	37,44,44	0.82	1 (2%)	40,65,65	1.36	3 (7%)
5	A1JCH	B	604[B]	-	37,44,44	0.83	1 (2%)	40,65,65	1.50	5 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1JCH	A	604[A]	-	-	4/11/56/56	0/5/5/5
5	A1JCH	A	604[B]	-	-	6/11/56/56	0/5/5/5
5	A1JCH	B	604[B]	-	-	6/11/56/56	0/5/5/5
5	A1JCH	B	604[A]	-	-	4/11/56/56	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604[A]	A1JCH	C10-N2	3.44	1.33	1.30
5	B	604[B]	A1JCH	C10-N2	3.44	1.33	1.30
5	A	604[A]	A1JCH	C10-N2	3.37	1.33	1.30
5	A	604[B]	A1JCH	C10-N2	3.37	1.33	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604[B]	A1JCH	N5-N6-N7	-5.39	106.01	109.53
5	A	604[A]	A1JCH	N5-N6-N7	-5.26	106.10	109.53
5	A	604[B]	A1JCH	N5-N6-N7	-5.24	106.11	109.53
5	B	604[A]	A1JCH	N5-N6-N7	-5.13	106.18	109.53
5	A	604[A]	A1JCH	C19-N5-N6	4.76	109.14	104.33
5	B	604[B]	A1JCH	C19-N5-N6	4.75	109.13	104.33
5	B	604[A]	A1JCH	C19-N5-N6	4.71	109.09	104.33
5	A	604[B]	A1JCH	C19-N5-N6	4.67	109.04	104.33
5	A	604[B]	A1JCH	C-C1-C17	2.76	115.88	110.11
5	A	604[A]	A1JCH	C11-N4-C12	2.56	129.03	124.16
5	A	604[B]	A1JCH	C11-N4-C12	2.56	129.03	124.16
5	B	604[B]	A1JCH	O8-C18-C19	-2.45	103.98	110.95
5	B	604[A]	A1JCH	C10-N2-C9	-2.42	112.18	114.09
5	B	604[B]	A1JCH	C10-N2-C9	-2.42	112.18	114.09
5	A	604[A]	A1JCH	C10-N2-C9	-2.33	112.25	114.09
5	A	604[B]	A1JCH	C10-N2-C9	-2.33	112.25	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604[B]	A1JCH	C-C1-C17	2.14	114.58	110.11

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604[A]	A1JCH	O4-C2-C3-C6
5	A	604[A]	A1JCH	O4-C2-C3-O5
5	A	604[A]	A1JCH	C8-C11-N4-C12
5	A	604[A]	A1JCH	N3-C11-N4-C12
5	A	604[B]	A1JCH	O4-C2-C3-C6
5	A	604[B]	A1JCH	O4-C2-C3-O5
5	A	604[B]	A1JCH	C8-C11-N4-C12
5	A	604[B]	A1JCH	N3-C11-N4-C12
5	B	604[A]	A1JCH	O4-C2-C3-C6
5	B	604[A]	A1JCH	C8-C11-N4-C12
5	B	604[A]	A1JCH	N3-C11-N4-C12
5	B	604[B]	A1JCH	O4-C2-C3-C6
5	B	604[B]	A1JCH	C8-C11-N4-C12
5	B	604[B]	A1JCH	N3-C11-N4-C12
5	B	604[A]	A1JCH	O4-C2-C3-O5
5	B	604[B]	A1JCH	O4-C2-C3-O5
5	B	604[B]	A1JCH	C19-C18-O8-C17
5	A	604[B]	A1JCH	C19-C18-O8-C17
5	B	604[B]	A1JCH	C1-C17-O8-C18
5	A	604[B]	A1JCH	C1-C17-O8-C18

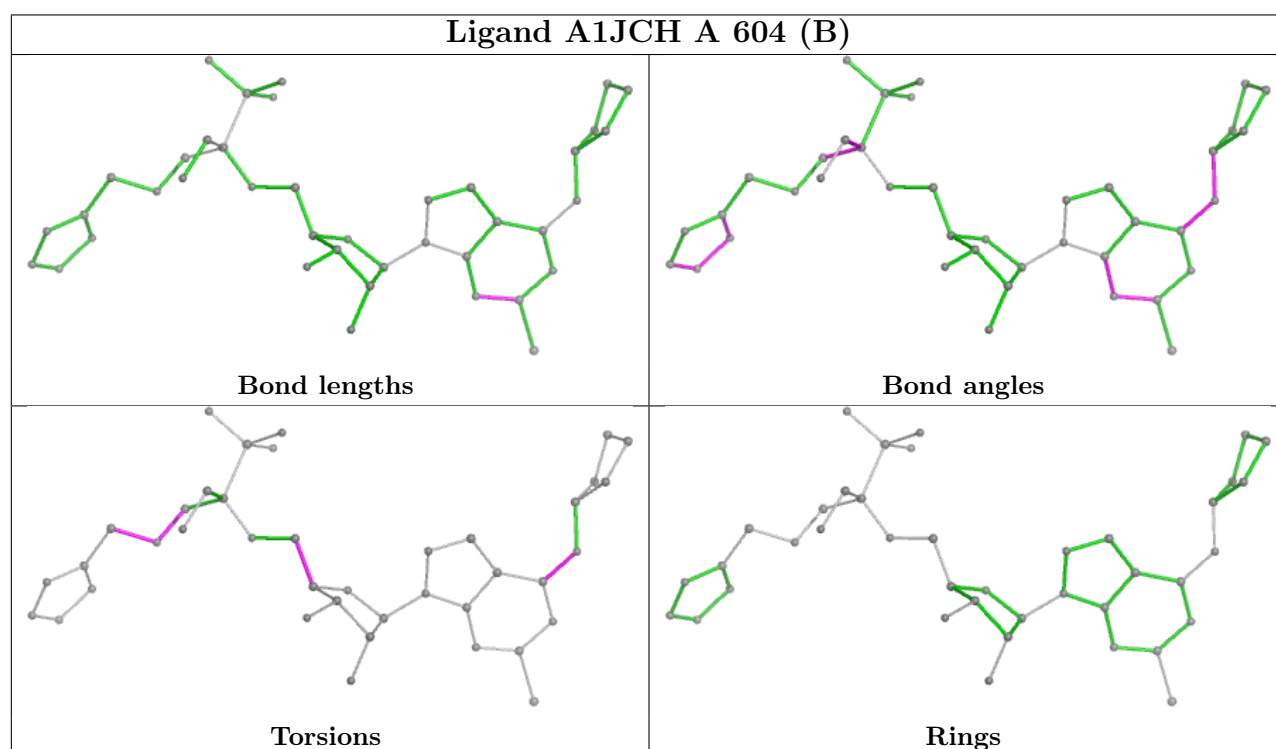
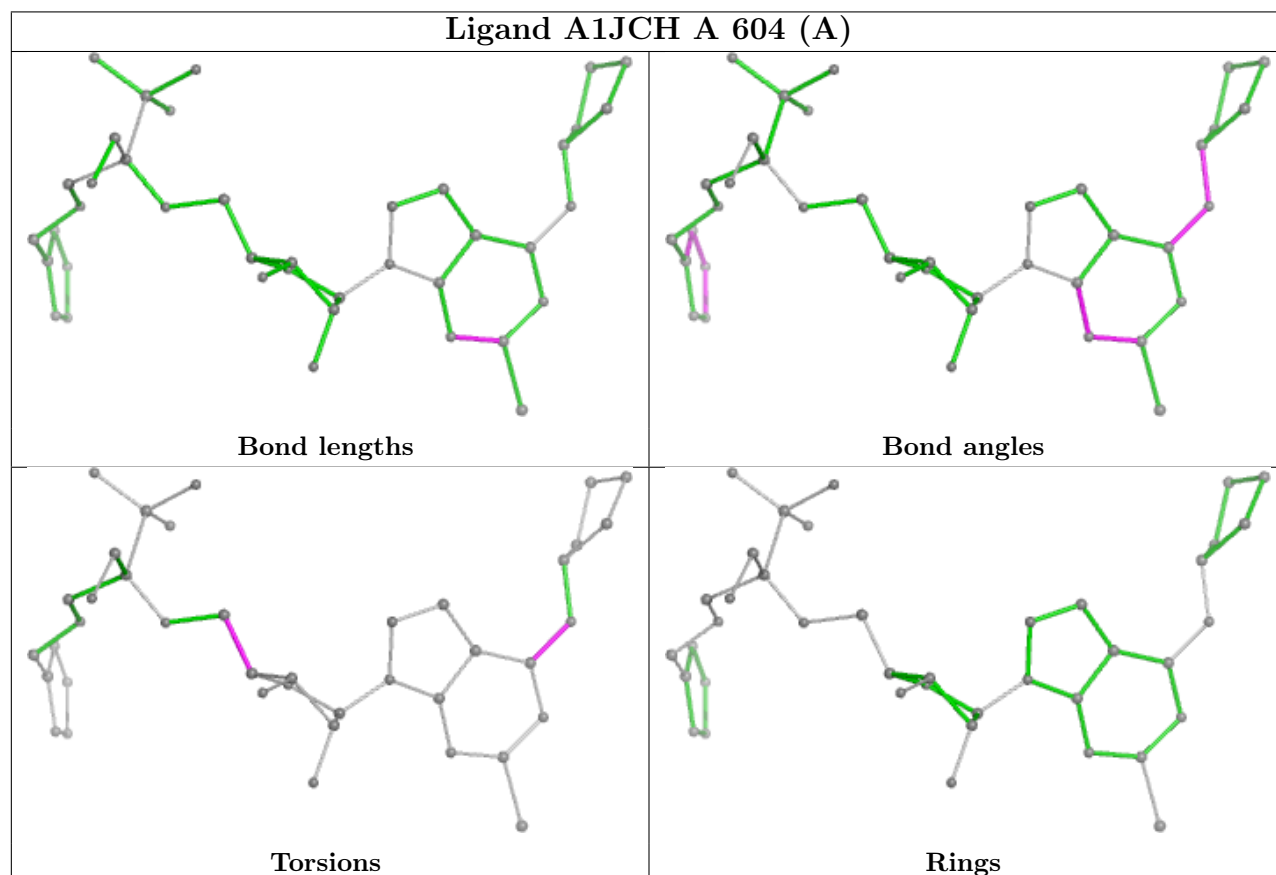
There are no ring outliers.

2 monomers are involved in 4 short contacts:

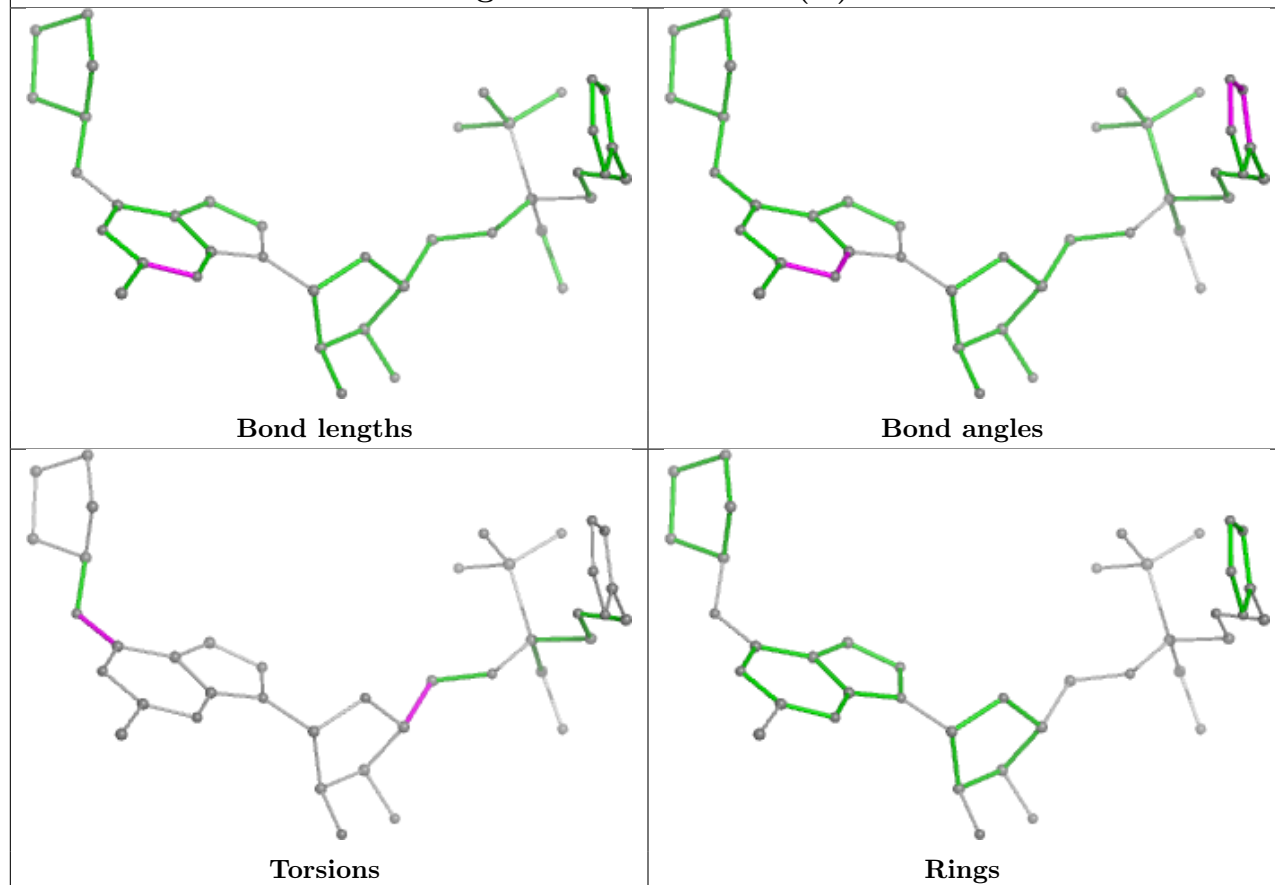
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604[B]	A1JCH	1	0
5	B	604[B]	A1JCH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

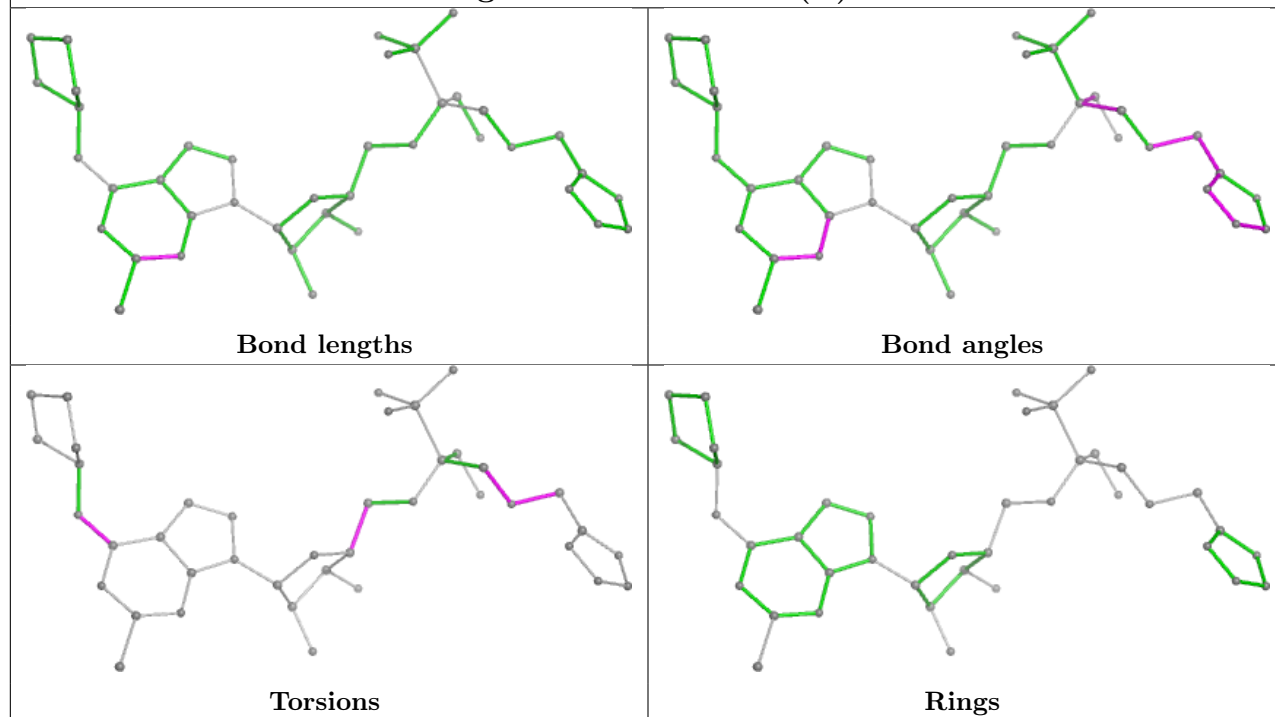
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand A1JCH B 604 (A)



Ligand A1JCH B 604 (B)



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	525/533 (98%)	-0.04	11 (2%) 63 64	16, 40, 70, 106	31 (5%)
1	B	525/533 (98%)	-0.04	8 (1%) 71 72	18, 41, 69, 109	26 (4%)
All	All	1050/1066 (98%)	-0.04	19 (1%) 67 68	16, 40, 69, 109	57 (5%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	MET	4.0
1	B	551	HIS	3.6
1	A	376	THR	3.6
1	B	374	ARG	3.6
1	A	378	GLU	3.3
1	B	403	ASP	3.2
1	B	550	HIS	3.1
1	B	379	MET	3.0
1	A	374	ARG	2.9
1	B	381	TRP	2.8
1	A	152	SER	2.7
1	B	337	GLN	2.6
1	A	403	ASP	2.3
1	B	375	HIS	2.3
1	A	256[A]	LYS	2.3
1	A	464	LYS	2.3
1	A	335	SER	2.0
1	A	477	THR	2.0
1	A	490	ASP	2.0

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

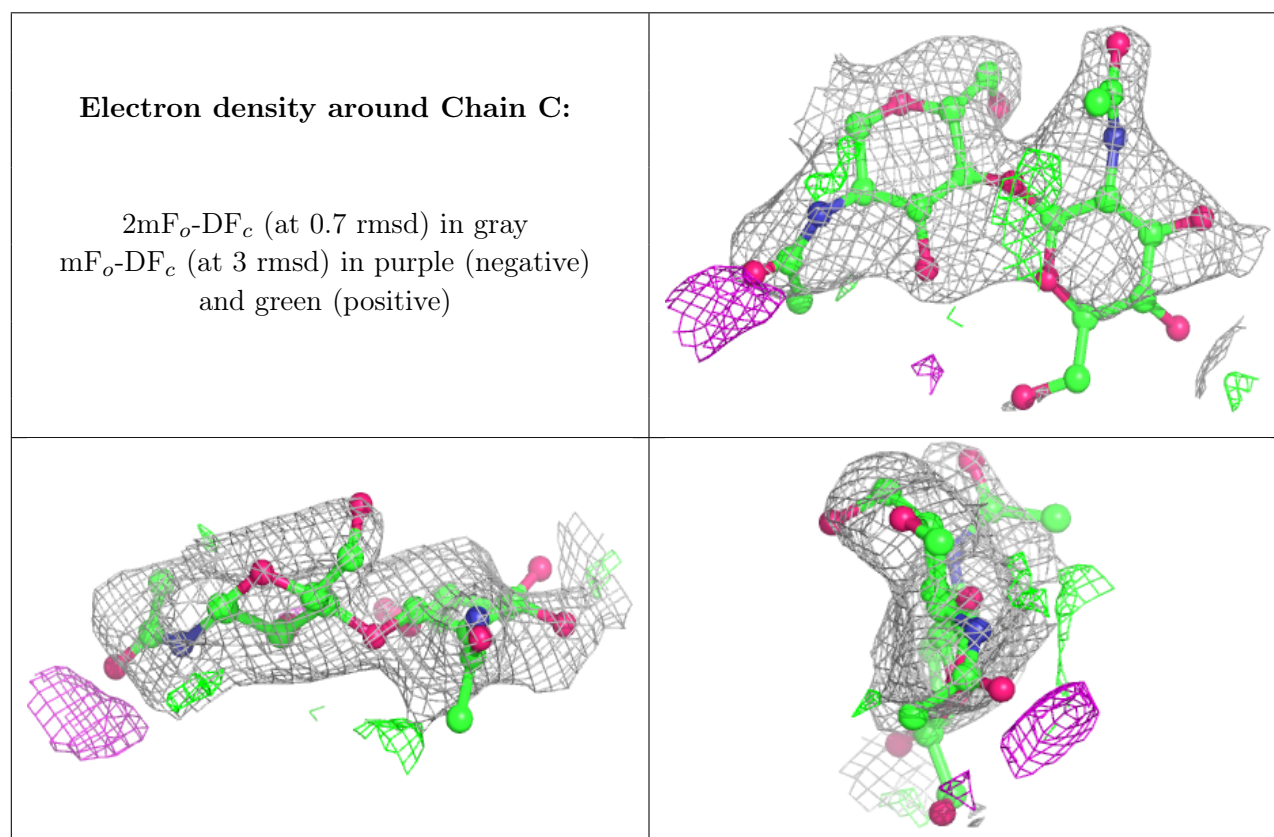
There are no non-standard protein/DNA/RNA residues in this entry.

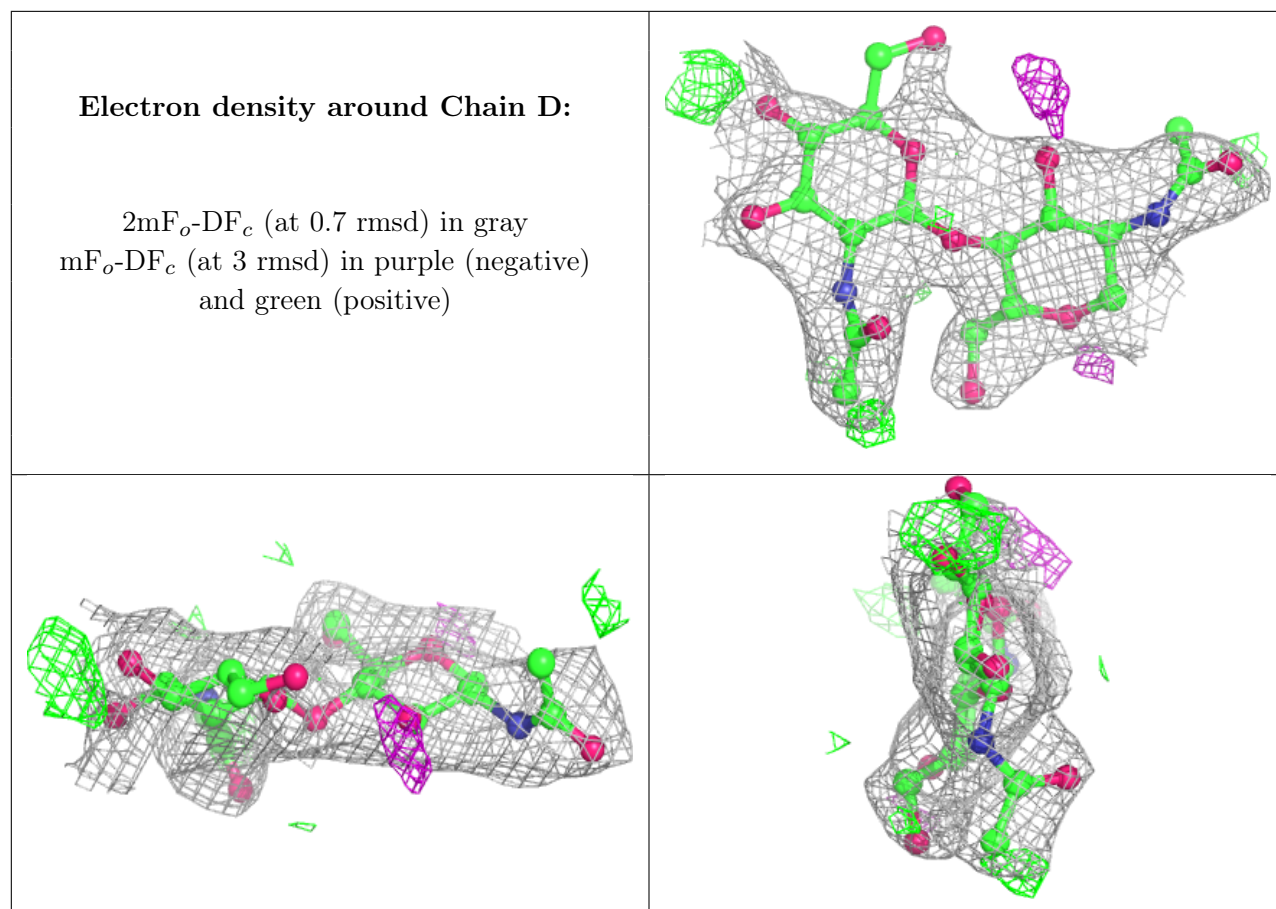
6.3 Carbohydrates ⓘ

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	D	2	14/15	0.62	0.17	63,85,104,105	0
2	NAG	C	2	14/15	0.63	0.18	82,97,130,145	0
2	NAG	C	1	14/15	0.81	0.17	41,64,86,89	0
2	NAG	D	1	14/15	0.88	0.12	35,52,68,72	0

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





6.4 Ligands ⓘ

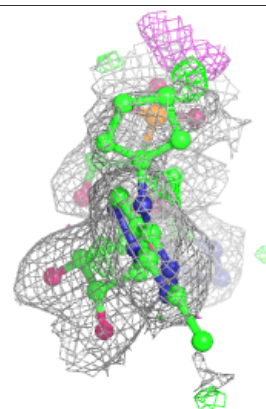
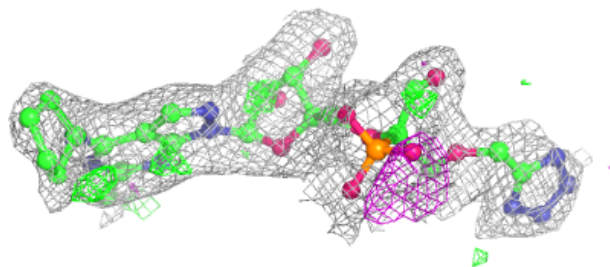
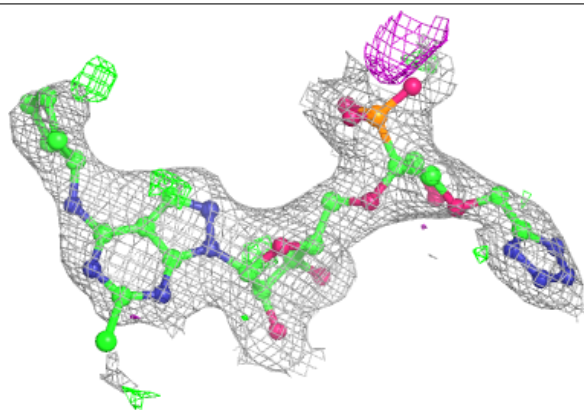
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	B	605	5/5	0.88	0.11	60,64,69,74	0
3	ZN	A	601	1/1	0.92	0.10	46,46,46,46	0
5	A1JCH	A	604[B]	40/40	0.93	0.12	26,41,86,121	8
5	A1JCH	B	604[A]	40/40	0.93	0.12	29,40,83,108	8
5	A1JCH	B	604[B]	40/40	0.93	0.12	28,39,83,108	8
6	PO4	A	605	5/5	0.93	0.12	48,63,69,70	0
5	A1JCH	A	604[A]	40/40	0.93	0.12	26,41,86,121	8
4	CA	A	603	1/1	0.94	0.06	32,32,32,32	1
4	CA	B	603	1/1	0.95	0.07	35,35,35,35	1
3	ZN	B	601	1/1	0.97	0.06	45,45,45,45	0
3	ZN	A	602	1/1	0.98	0.03	29,29,29,29	0
3	ZN	B	602	1/1	0.98	0.03	31,31,31,31	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.

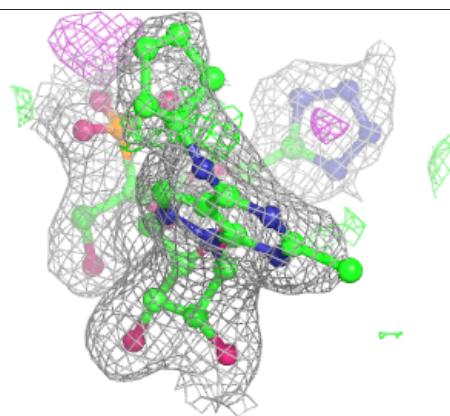
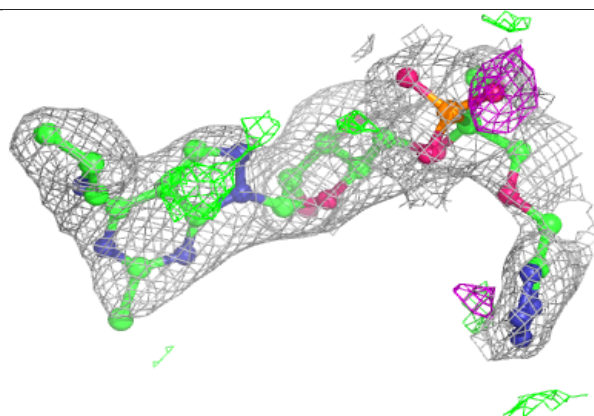
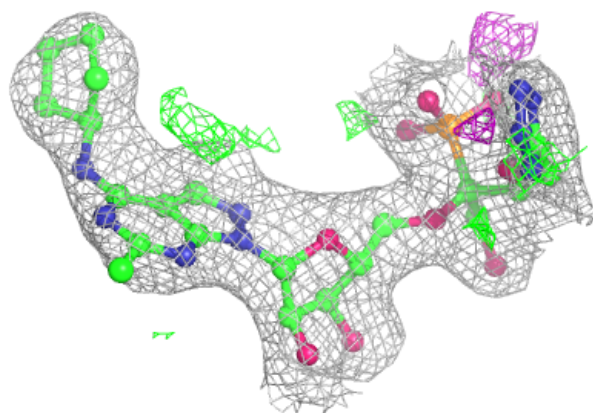
Electron density around A1JCH A 604 (B):

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

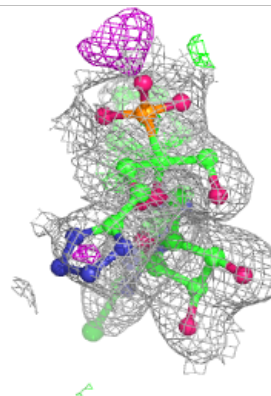
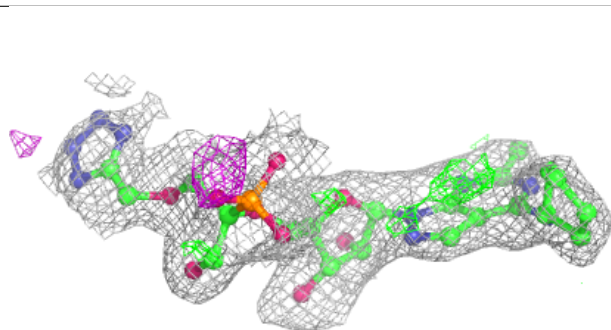
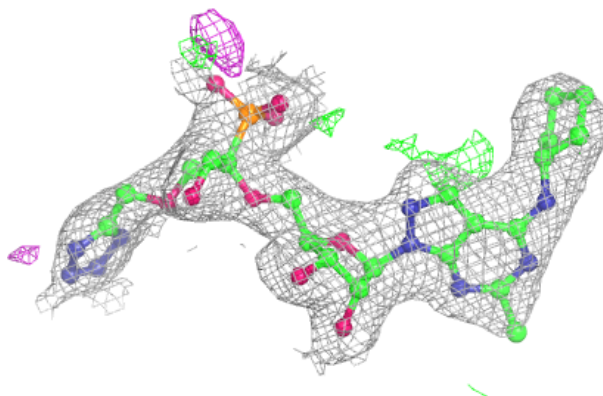


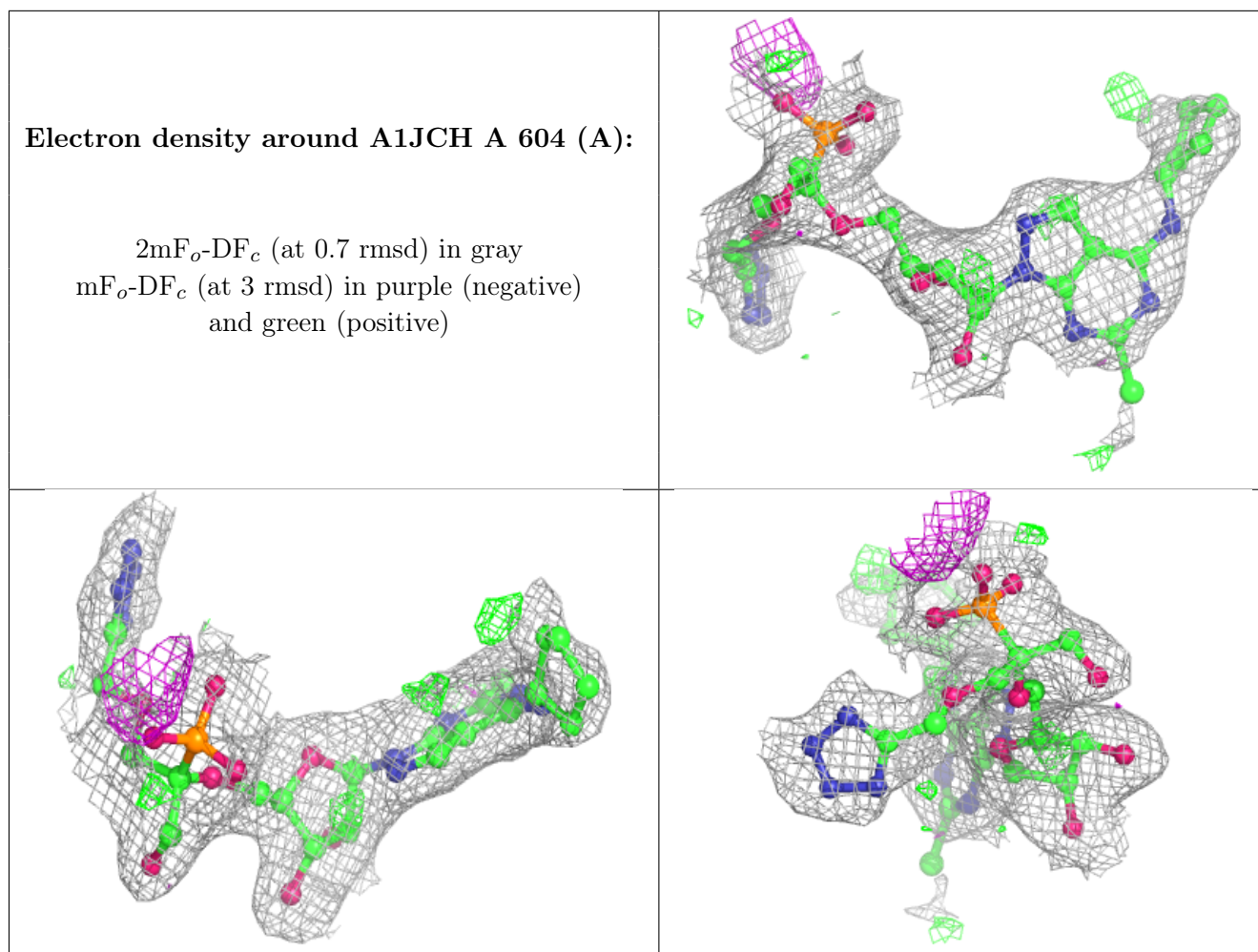
Electron density around A1JCH B 604 (A):

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

**Electron density around A1JCH B 604 (B):**

$2mF_o-DF_c$ (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.