



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2022 – 03:16 pm GMT

PDB ID : 7P4J
Title : Crystal structure of Autotaxin and tetrahydrocannabinol
Authors : Eymery, M.C.; McCarthy, A.A.; Hausmann, J.
Deposited on : 2021-07-11
Resolution : 1.79 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

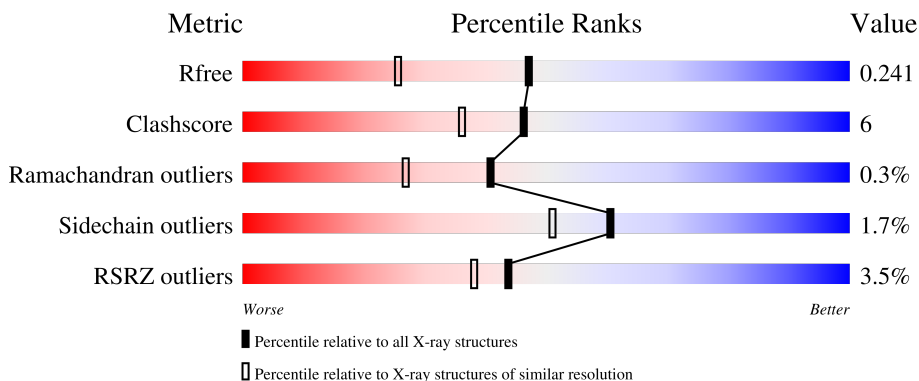
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	827	
2	B	2	

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 6792 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	770	6222	3950	1073	1150	49	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	581	PHE	LEU	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	806	ALA	ASN	engineered mutation	UNP Q64610

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

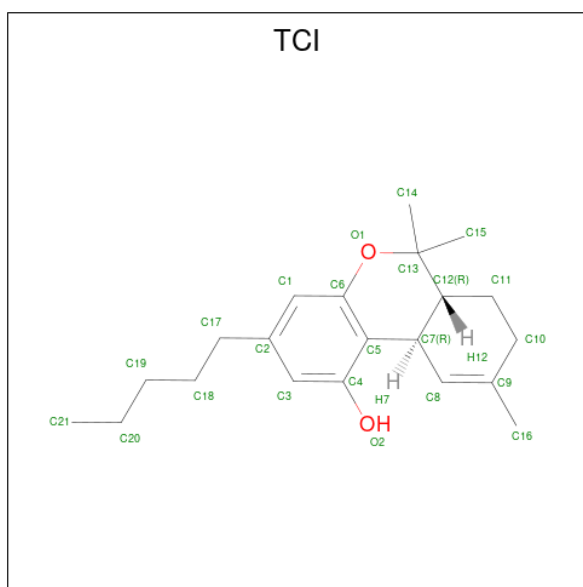


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

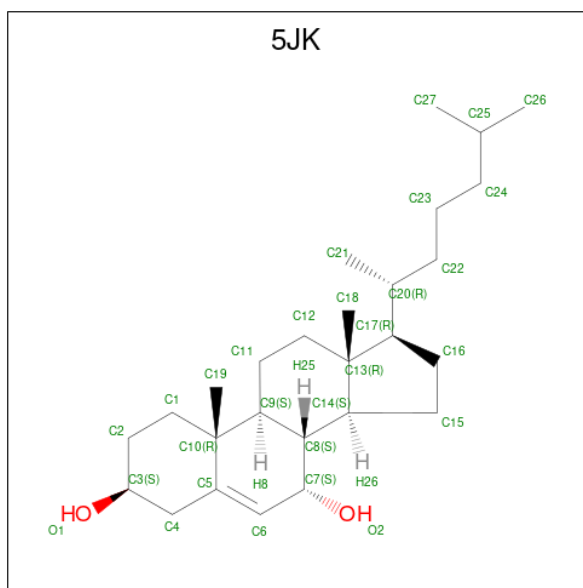
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (6aR,10aR)-6,6,9-trimethyl-3-pentyl-6a,7,8,10a-tetrahydro-6H-benzo[c]chromen-1-ol (three-letter code: TCI) (formula: C₂₁H₃₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	C	O	0	0
			23	21	2		

- Molecule 5 is 7 α -hydroxycholesterol (three-letter code: 5JK) (formula: C₂₇H₄₆O₂).

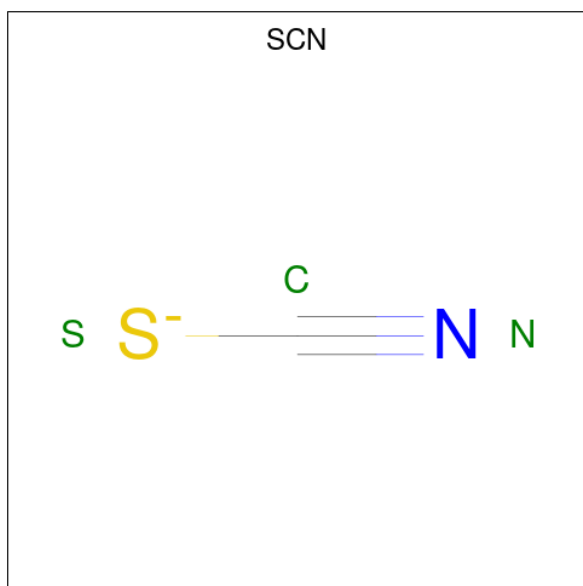


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	A	1	Total	C	O	0	0
			29	27	2		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

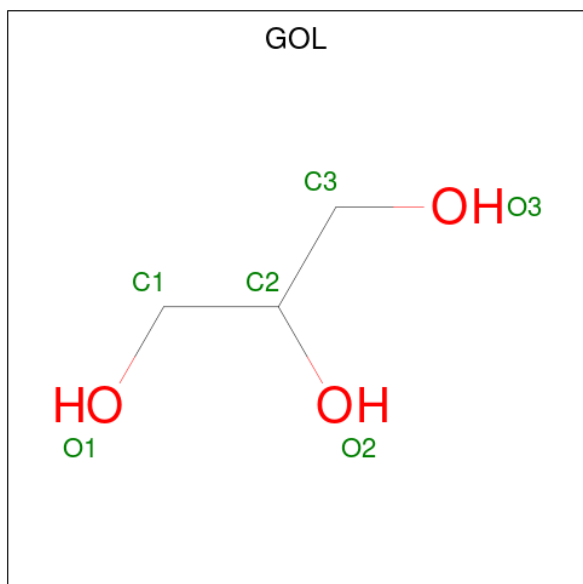
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	19	Total I 19 19	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



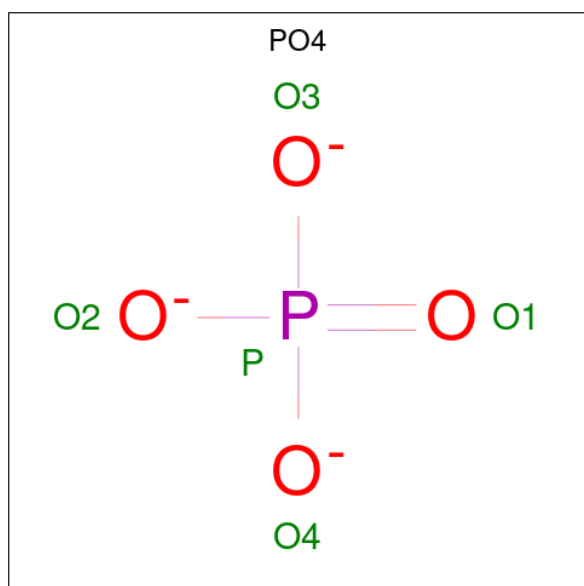
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Ca 2 2	0	0

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Na 1 1	0	0

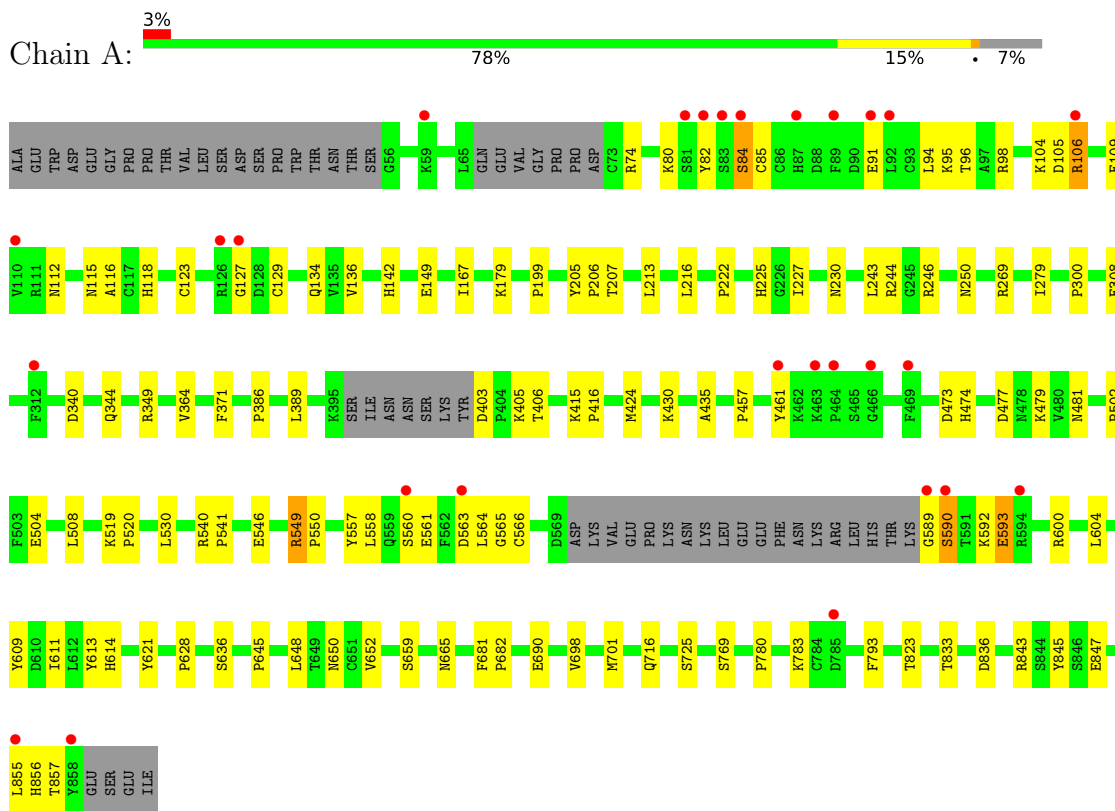
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	407	Total O 407 407	0	0

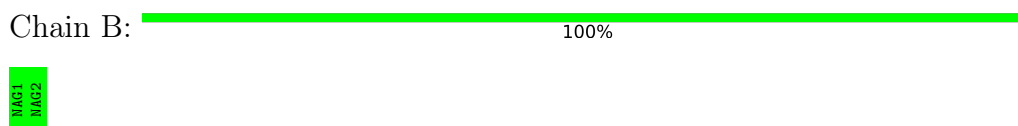
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- 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 1	Depositor
Cell constants a, b, c, α , β , γ	53.70Å 60.98Å 63.60Å 103.15° 97.39° 94.23°	Depositor
Resolution (Å)	61.24 – 1.79 61.24 – 1.79	Depositor EDS
% Data completeness (in resolution range)	65.9 (61.24-1.79) 65.9 (61.24-1.79)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.183 , 0.241 0.183 , 0.241	Depositor DCC
R_{free} test set	2005 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SCN, PO4, NAG, NA, GOL, CA, TCI, IOD, 5JK

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	0.42	0/6398	0.60	2/8674 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	540	ARG	NE-CZ-NH1	5.83	123.21	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	590	SER	Peptide
1	A	593	GLU	Peptide
1	A	82	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6222	0	5984	78	1
2	B	28	0	25	0	0
3	A	2	0	0	0	0
4	A	23	0	29	3	0
5	A	29	0	0	0	0
6	A	19	0	0	2	0
7	A	6	0	0	0	0
8	A	48	0	64	7	0
9	A	5	0	0	0	0
10	A	2	0	0	0	0
11	A	1	0	0	0	0
12	A	407	0	0	5	1
All	All	6792	0	6102	79	2

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 6.

All (79) 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:592:LYS:HD3	1:A:613:TYR:HB3	1.49	0.94
1:A:134:GLN:OE1	1:A:344:GLN:NE2	2.04	0.89
1:A:558:LEU:N	1:A:561:GLU:OE1	2.17	0.73
1:A:564:LEU:HB2	6:A:926:IOD:I	2.60	0.72
1:A:519:LYS:NZ	12:A:1002:HOH:O	2.23	0.71
1:A:179:LYS:HE3	1:A:179:LYS:HA	1.78	0.66
1:A:650:ASN:HB3	8:A:914:GOL:H11	1.80	0.62
1:A:519:LYS:HD3	1:A:520:PRO:HD2	1.81	0.62
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.82	0.62
1:A:213:LEU:HD13	4:A:903:TCI:H7	1.81	0.61
1:A:592:LYS:HG2	1:A:614:HIS:O	2.00	0.60
1:A:690:GLU:OE1	1:A:690:GLU:N	2.30	0.60
1:A:216:LEU:HD13	4:A:903:TCI:H20A	1.86	0.58
1:A:481:ASN:ND2	12:A:1014:HOH:O	2.37	0.58
1:A:430:LYS:HA	8:A:912:GOL:H31	1.86	0.58
1:A:564:LEU:HA	1:A:665:ASN:HB2	1.85	0.57
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.87	0.57
1:A:833:THR:HB	8:A:918:GOL:H32	1.87	0.57
1:A:230:ASN:HB3	1:A:243:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:CD	1:A:600:ARG:HH12	2.09	0.56
1:A:403:ASP:HB3	1:A:406:THR:HB	1.88	0.55
1:A:94:LEU:HD21	1:A:279:ILE:HD12	1.89	0.54
1:A:604:LEU:HD11	1:A:836:ASP:HB2	1.90	0.54
1:A:98:ARG:HB2	12:A:1258:HOH:O	2.09	0.53
1:A:550:PRO:HB3	1:A:609:TYR:CZ	2.44	0.53
1:A:349:ARG:NH1	12:A:1018:HOH:O	2.42	0.53
1:A:769:SER:HB2	1:A:793:PHE:CZ	2.44	0.52
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.43	0.52
1:A:142:HIS:ND1	1:A:340:ASP:OD2	2.38	0.52
1:A:530:LEU:HB2	8:A:916:GOL:H2	1.92	0.51
1:A:563:ASP:O	1:A:565:GLY:N	2.38	0.51
1:A:589:GLY:HA3	1:A:592:LYS:HD2	1.92	0.51
1:A:91:GLU:O	1:A:95:LYS:HG2	2.11	0.51
1:A:504:GLU:HB3	12:A:1107:HOH:O	2.11	0.50
1:A:118:HIS:O	1:A:129:CYS:HA	2.11	0.50
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.46	0.50
1:A:780:PRO:HG2	1:A:783:LYS:HB2	1.93	0.49
1:A:167:ILE:HG21	4:A:903:TCI:H21B	1.94	0.49
1:A:823:THR:HG23	1:A:855:LEU:HD11	1.94	0.49
1:A:149:GLU:HB3	1:A:349:ARG:HH12	1.77	0.49
1:A:364:VAL:HG21	1:A:473:ASP:HB2	1.94	0.49
1:A:725:SER:O	8:A:913:GOL:O2	2.28	0.48
1:A:590:SER:HA	1:A:593:GLU:HG2	1.94	0.48
1:A:549:ARG:HG2	1:A:550:PRO:HD2	1.95	0.48
1:A:645:PRO:HG2	1:A:648:LEU:HD12	1.95	0.47
1:A:592:LYS:CD	1:A:613:TYR:HB3	2.34	0.47
1:A:681:PHE:CD1	1:A:682:PRO:HD2	2.49	0.47
1:A:106:ARG:HD2	1:A:109:GLU:HB3	1.97	0.47
1:A:698:VAL:HG23	1:A:701:MET:HE2	1.97	0.47
1:A:541:PRO:HB2	1:A:845:TYR:CE2	2.50	0.46
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.98	0.46
1:A:207:THR:O	1:A:474:HIS:HD2	1.99	0.46
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.51	0.46
1:A:96:THR:HA	1:A:116:ALA:HB2	1.97	0.45
1:A:106:ARG:HD2	1:A:109:GLU:CB	2.47	0.45
1:A:80:LYS:HG2	1:A:85:CYS:SG	2.56	0.45
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.99	0.45
1:A:123:CYS:O	1:A:127:GLY:N	2.51	0.44
1:A:104:LYS:HG3	1:A:136:VAL:CG1	2.48	0.43
1:A:104:LYS:HG3	1:A:136:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:HH12	1:A:550:PRO:HG2	1.83	0.43
1:A:405:LYS:HE2	1:A:424:MET:HG3	2.01	0.43
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.75	0.42
1:A:549:ARG:NH1	1:A:550:PRO:HG2	2.35	0.42
1:A:477:ASP:HB2	8:A:919:GOL:H32	2.00	0.42
1:A:855:LEU:HD23	1:A:857:THR:HG22	2.02	0.42
1:A:557:TYR:OH	1:A:659:SER:HB2	2.20	0.42
1:A:112:ASN:HB3	1:A:115:ASN:OD1	2.19	0.41
1:A:589:GLY:CA	1:A:592:LYS:HD2	2.49	0.41
1:A:225:HIS:CE1	1:A:227:ILE:HB	2.55	0.41
1:A:74:ARG:O	1:A:85:CYS:HA	2.20	0.41
1:A:415:LYS:HG3	1:A:416:PRO:HD2	2.02	0.41
6:A:931:IOD:I	6:A:932:IOD:I	3.78	0.41
1:A:621:TYR:HA	1:A:628:PRO:HA	2.03	0.41
1:A:843:ARG:NE	1:A:847:GLU:OE2	2.36	0.41
1:A:308:GLU:H	1:A:308:GLU:CD	2.24	0.41
1:A:435:ALA:HB2	8:A:912:GOL:H2	2.03	0.41
1:A:566:CYS:HB3	1:A:652:VAL:HB	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:OE2	1:A:549:ARG:NH2[1_656]	1.87	0.33
12:A:1270:HOH:O	12:A:1321:HOH:O[1_666]	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	763/827 (92%)	733 (96%)	28 (4%)	2 (0%)	41 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	386	PRO

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	696/749 (93%)	684 (98%)	12 (2%)	60 51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	105	ASP
1	A	106	ARG
1	A	244	ARG
1	A	246	ARG
1	A	389	LEU
1	A	461	TYR
1	A	479	LYS
1	A	549	ARG
1	A	560	SER
1	A	636	SER
1	A	856	HIS

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

Mol	Chain	Res	Type
1	A	326	ASN
1	A	474	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	2,1	14,14,15	0.29	0	17,19,21	0.63	0
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	0.35	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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

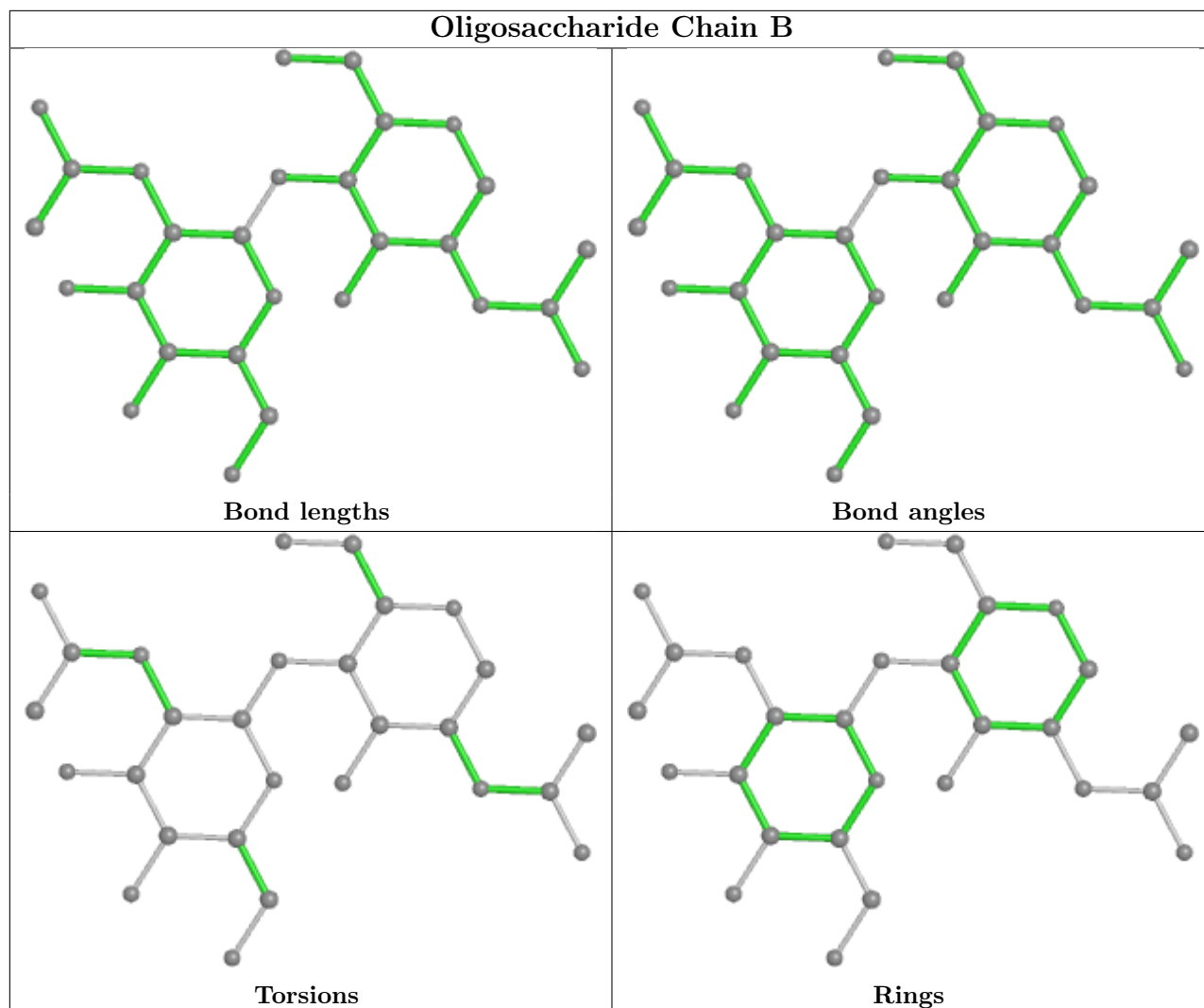
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 37 ligands modelled in this entry, 24 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TCI	A	903	-	25,25,25	0.29	0	32,37,37	0.67	1 (3%)
8	GOL	A	910	-	5,5,5	0.87	0	5,5,5	0.93	0
8	GOL	A	916	-	5,5,5	0.94	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SCN	A	917	-	1,2,2	1.37	0	0,1,1	-	-
8	GOL	A	914	-	5,5,5	0.75	0	5,5,5	0.97	0
8	GOL	A	912	-	5,5,5	1.34	1 (20%)	5,5,5	1.01	0
8	GOL	A	913	-	5,5,5	0.57	0	5,5,5	0.99	0
8	GOL	A	918	-	5,5,5	0.98	0	5,5,5	1.19	0
7	SCN	A	909	-	1,2,2	0.72	0	0,1,1	-	-
5	5JK	A	904	-	32,32,32	3.91	12 (37%)	47,50,50	3.28	13 (27%)
8	GOL	A	919	-	5,5,5	0.60	0	5,5,5	1.04	0
8	GOL	A	911	-	5,5,5	1.08	0	5,5,5	0.67	0
9	PO4	A	915	3	4,4,4	0.69	0	6,6,6	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TCI	A	903	-	-	3/5/33/33	0/3/3/3
8	GOL	A	910	-	-	3/4/4/4	-
8	GOL	A	916	-	-	1/4/4/4	-
8	GOL	A	914	-	-	2/4/4/4	-
8	GOL	A	912	-	-	2/4/4/4	-
8	GOL	A	913	-	-	3/4/4/4	-
8	GOL	A	918	-	-	2/4/4/4	-
5	5JK	A	904	-	-	0/10/71/71	0/4/4/4
8	GOL	A	919	-	-	0/4/4/4	-
8	GOL	A	911	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	5JK	C6-C5	13.67	1.57	1.33
5	A	904	5JK	C8-C7	8.02	1.62	1.53
5	A	904	5JK	C16-C15	6.36	1.71	1.54
5	A	904	5JK	C20-C17	-6.16	1.43	1.54
5	A	904	5JK	C13-C17	5.56	1.65	1.55
5	A	904	5JK	C15-C14	5.51	1.65	1.54
5	A	904	5JK	C12-C11	4.41	1.62	1.53
5	A	904	5JK	C12-C13	-3.75	1.47	1.54
5	A	904	5JK	O2-C7	-3.26	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	5JK	C10-C9	3.19	1.61	1.56
5	A	904	5JK	C8-C9	2.81	1.59	1.53
5	A	904	5JK	C8-C14	-2.40	1.49	1.53
8	A	912	GOL	O2-C2	-2.12	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	5JK	C7-C6-C5	-18.40	113.45	125.42
5	A	904	5JK	C16-C17-C20	-4.15	105.72	112.15
5	A	904	5JK	C22-C20-C17	-4.13	101.75	110.28
5	A	904	5JK	C17-C13-C14	3.97	104.78	100.07
5	A	904	5JK	C12-C13-C17	3.73	122.15	116.57
5	A	904	5JK	C18-C13-C12	-3.66	104.81	110.59
5	A	904	5JK	C1-C10-C5	3.29	114.78	108.75
5	A	904	5JK	C18-C13-C14	-3.22	105.72	111.71
5	A	904	5JK	C12-C13-C14	2.73	111.51	107.27
5	A	904	5JK	C19-C10-C9	-2.69	108.47	111.68
5	A	904	5JK	C18-C13-C17	-2.66	106.76	111.71
5	A	904	5JK	C16-C17-C13	2.50	106.85	103.84
4	A	903	TCI	O1-C13-C12	2.24	114.60	109.27
5	A	904	5JK	C10-C5-C6	-2.24	119.47	122.81

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	910	GOL	C1-C2-C3-O3
8	A	912	GOL	O1-C1-C2-C3
8	A	913	GOL	O1-C1-C2-C3
8	A	914	GOL	C1-C2-C3-O3
8	A	913	GOL	O1-C1-C2-O2
8	A	914	GOL	O2-C2-C3-O3
8	A	918	GOL	O1-C1-C2-C3
8	A	910	GOL	O2-C2-C3-O3
8	A	912	GOL	O1-C1-C2-O2
4	A	903	TCI	C18-C19-C20-C21
8	A	913	GOL	O2-C2-C3-O3
8	A	916	GOL	O2-C2-C3-O3
4	A	903	TCI	C2-C17-C18-C19
8	A	910	GOL	O1-C1-C2-C3
8	A	918	GOL	O1-C1-C2-O2

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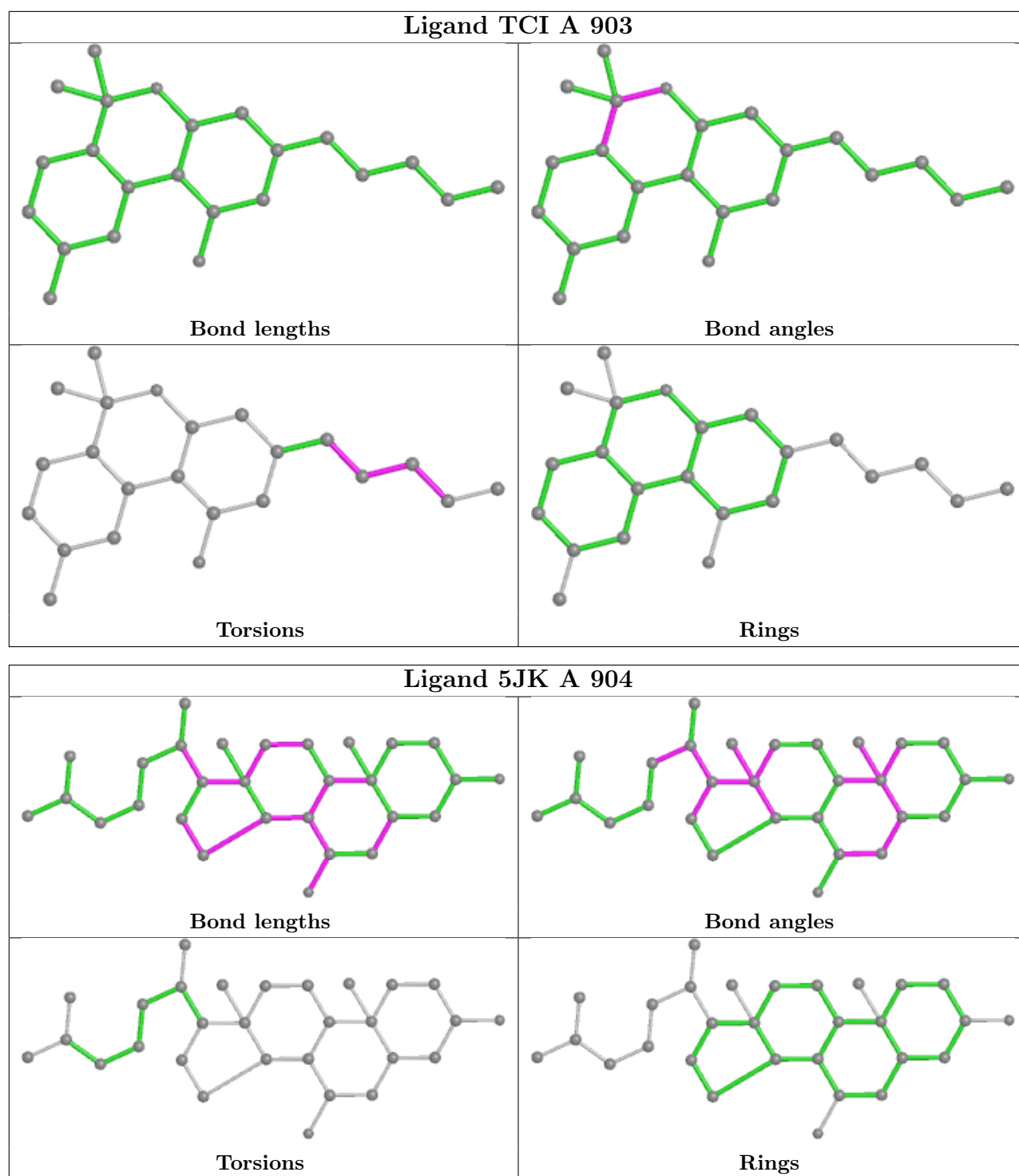
Mol	Chain	Res	Type	Atoms
4	A	903	TCI	C17-C18-C19-C20

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	TCI	3	0
8	A	916	GOL	1	0
8	A	914	GOL	1	0
8	A	912	GOL	2	0
8	A	913	GOL	1	0
8	A	918	GOL	1	0
8	A	919	GOL	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.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	770/827 (93%)	0.01	27 (3%) 44 38	10, 22, 43, 57	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	TYR	5.8
1	A	469	PHE	5.3
1	A	83	SER	4.9
1	A	464	PRO	4.3
1	A	590	SER	3.9
1	A	126	ARG	3.6
1	A	466	GLY	3.5
1	A	855	LEU	3.4
1	A	563	ASP	3.2
1	A	82	TYR	3.2
1	A	110	VAL	3.0
1	A	463	LYS	2.9
1	A	127	GLY	2.8
1	A	312	PHE	2.7
1	A	858	TYR	2.6
1	A	106	ARG	2.5
1	A	87	HIS	2.4
1	A	89	PHE	2.4
1	A	785	ASP	2.3
1	A	81	SER	2.3
1	A	560	SER	2.3
1	A	594	ARG	2.2
1	A	84	SER	2.2
1	A	59	LYS	2.2
1	A	91	GLU	2.2
1	A	92	LEU	2.0
1	A	589	GLY	2.0

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

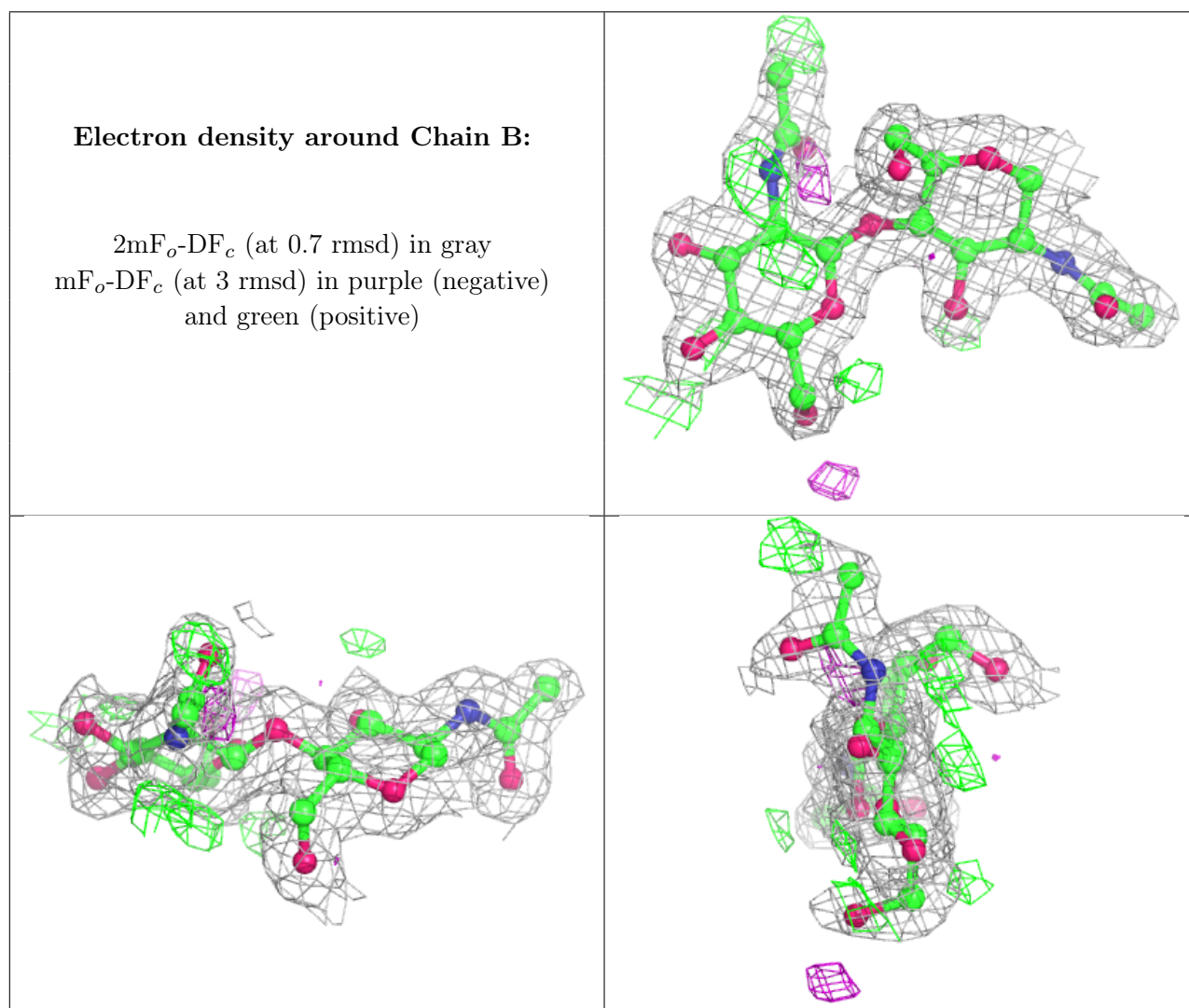
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.82	0.13	30,32,42,46	0
2	NAG	B	1	14/15	0.97	0.07	13,18,21,23	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.

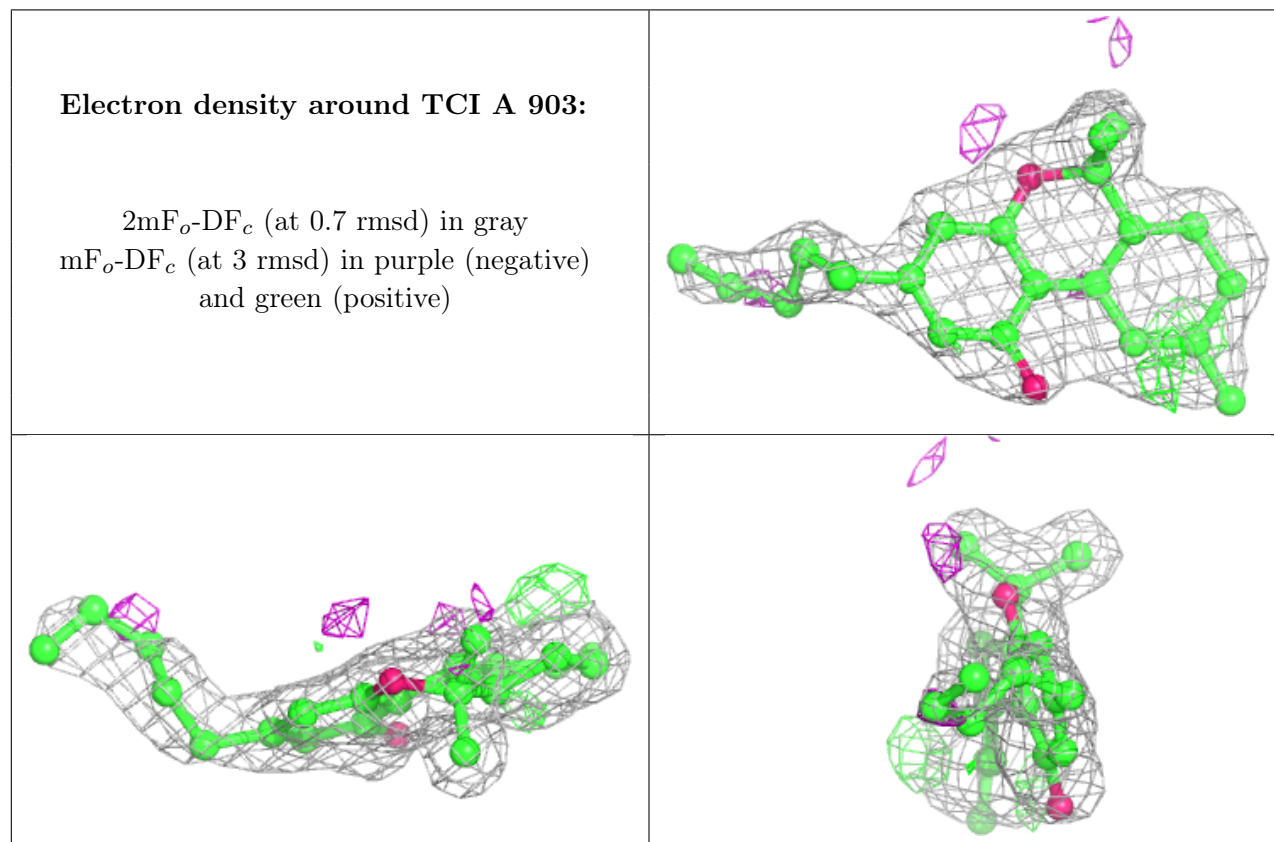


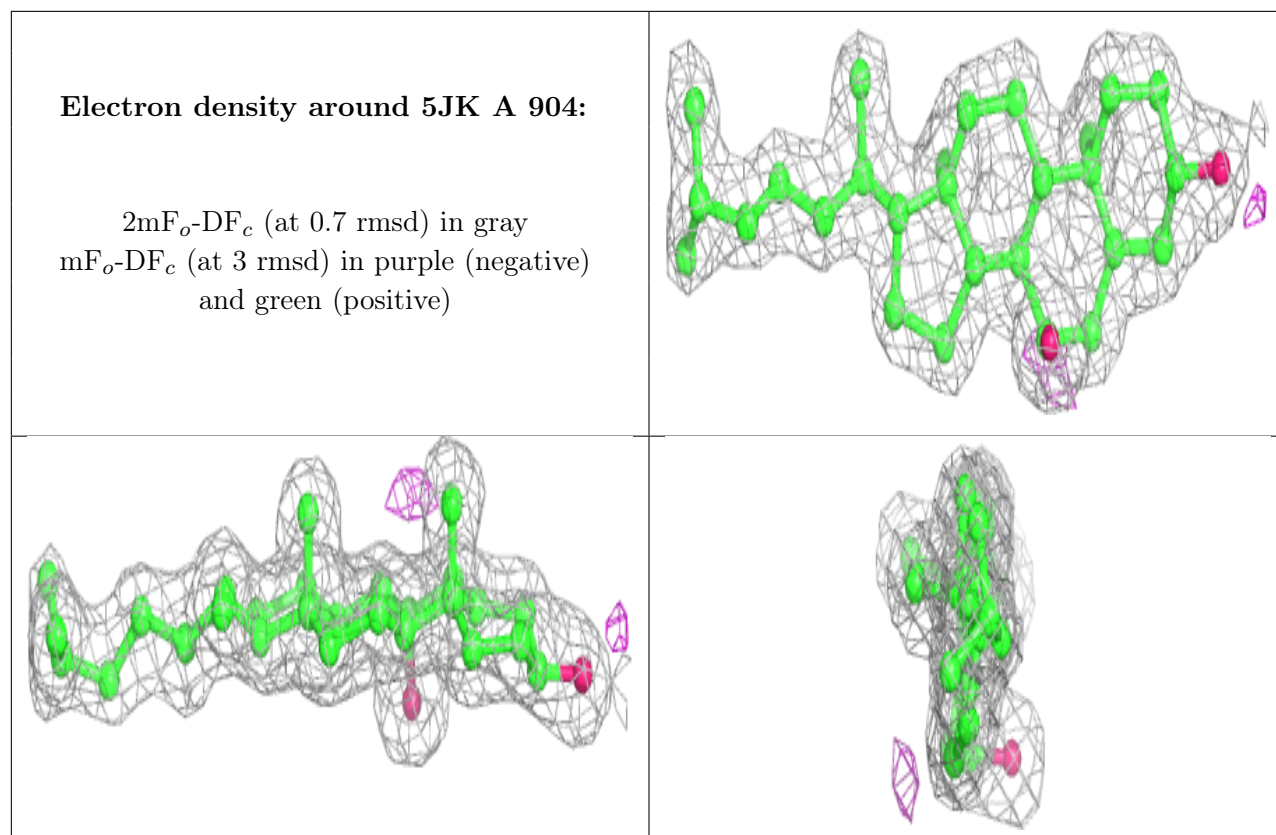
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
8	GOL	A	910	6/6	0.56	0.34	50,53,59,59	0
9	PO4	A	915	5/5	0.69	0.18	23,30,43,57	0
8	GOL	A	914	6/6	0.84	0.20	32,34,45,49	0
7	SCN	A	917	3/3	0.87	0.20	13,13,28,69	0
8	GOL	A	911	6/6	0.87	0.25	27,30,34,36	0
8	GOL	A	918	6/6	0.89	0.36	23,28,29,30	0
4	TCI	A	903	23/23	0.90	0.16	17,29,37,40	0
6	IOD	A	925	1/1	0.90	0.09	118,118,118,118	0
6	IOD	A	927	1/1	0.90	0.14	117,117,117,117	0
8	GOL	A	919	6/6	0.91	0.10	29,34,41,42	0
7	SCN	A	909	3/3	0.93	0.08	34,34,36,46	0
6	IOD	A	931	1/1	0.93	0.04	64,64,64,64	1
8	GOL	A	916	6/6	0.94	0.13	16,23,25,30	0
8	GOL	A	912	6/6	0.94	0.14	17,24,26,29	0
8	GOL	A	913	6/6	0.95	0.09	21,24,26,28	0
5	5JK	A	904	29/29	0.95	0.09	11,18,23,30	0
6	IOD	A	920	1/1	0.96	0.07	89,89,89,89	0
6	IOD	A	934	1/1	0.97	0.06	54,54,54,54	1
6	IOD	A	908	1/1	0.97	0.06	108,108,108,108	0
6	IOD	A	922	1/1	0.98	0.07	33,33,33,33	1
6	IOD	A	926	1/1	0.98	0.03	50,50,50,50	0
6	IOD	A	932	1/1	0.98	0.08	37,37,37,37	1
10	CA	A	936	1/1	0.98	0.04	49,49,49,49	0
11	NA	A	937	1/1	0.98	0.16	14,14,14,14	0
6	IOD	A	921	1/1	0.99	0.08	38,38,38,38	1
3	ZN	A	902	1/1	0.99	0.06	16,16,16,16	1
6	IOD	A	928	1/1	0.99	0.06	31,31,31,31	1
6	IOD	A	929	1/1	0.99	0.06	41,41,41,41	1
6	IOD	A	923	1/1	0.99	0.09	33,33,33,33	1
6	IOD	A	905	1/1	0.99	0.12	21,21,21,21	1
6	IOD	A	933	1/1	0.99	0.02	73,73,73,73	1
6	IOD	A	924	1/1	1.00	0.13	17,17,17,17	1
6	IOD	A	907	1/1	1.00	0.10	25,25,25,25	1
6	IOD	A	930	1/1	1.00	0.12	18,18,18,18	1
10	CA	A	935	1/1	1.00	0.10	15,15,15,15	0
3	ZN	A	901	1/1	1.00	0.09	16,16,16,16	1
6	IOD	A	906	1/1	1.00	0.12	16,16,16,16	1

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





6.5 Other polymers [i](#)

There are no such residues in this entry.