



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:43 AM BST

PDB ID : 5L0E
Title : Crystal Structure of Autotaxin and Compound 1
Authors : Durbin, J.D.
Deposited on : 2016-07-27
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

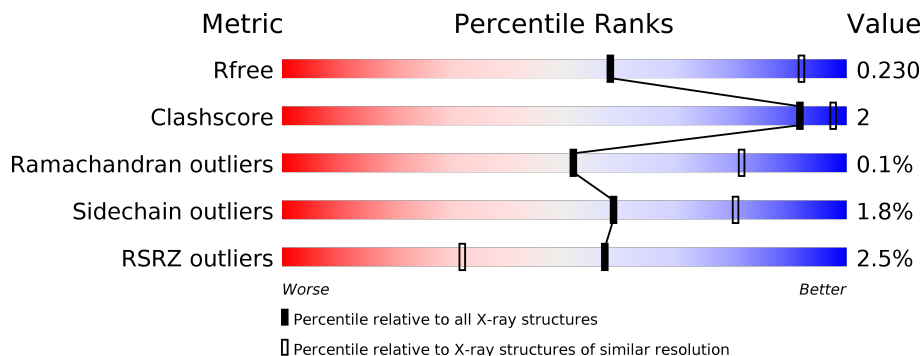
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	871	<p>3% 85% 5% 10%</p>
1	B	871	<p>2% 84% 6% 10%</p>
2	C	9	<p>22% 78%</p>
3	D	6	<p>33% 67%</p>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12992 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.

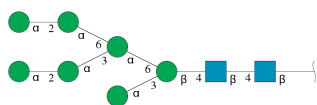
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	783	6319	4001	1088	1181	49	0	0	0
1	B	782	6310	3995	1086	1180	49	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	591	THR	ARG	engineered mutation	UNP Q64610
A	592	GLU	LYS	engineered mutation	UNP Q64610
A	863	ALA	-	expression tag	UNP Q64610
A	864	ALA	-	expression tag	UNP Q64610
A	865	ALA	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
B	591	THR	ARG	engineered mutation	UNP Q64610
B	592	GLU	LYS	engineered mutation	UNP Q64610
B	863	ALA	-	expression tag	UNP Q64610
B	864	ALA	-	expression tag	UNP Q64610
B	865	ALA	-	expression tag	UNP Q64610
B	866	HIS	-	expression tag	UNP Q64610
B	867	HIS	-	expression tag	UNP Q64610
B	868	HIS	-	expression tag	UNP Q64610
B	869	HIS	-	expression tag	UNP Q64610
B	870	HIS	-	expression tag	UNP Q64610
B	871	HIS	-	expression tag	UNP Q64610

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



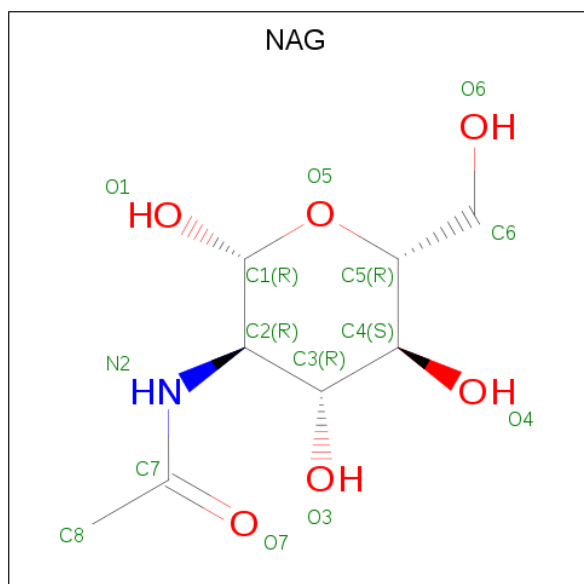
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	9	105	58	2	45	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



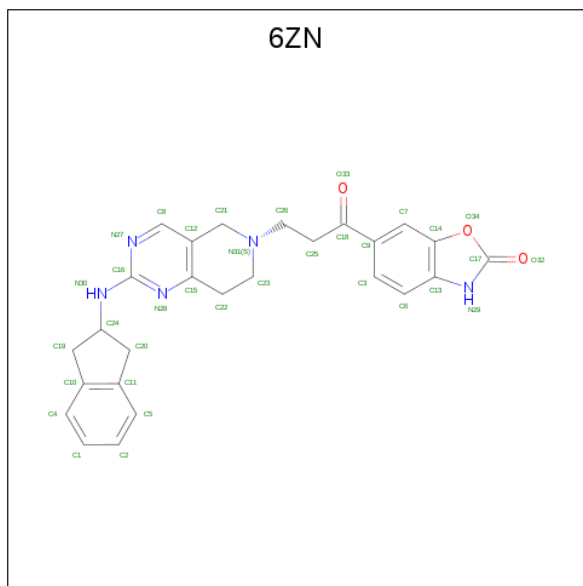
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	6	72	40	2	30	0	0	0

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



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

- Molecule 5 is 6-(3-{2-[(2,3-dihydro-1H-inden-2-yl)amino]-7,8-dihydropyrido[4,3-d]pyrimidin-6(5H)-yl}propanoyl)-1,3-benzoxazol-2(3H)-one (three-letter code: 6ZN) (formula: C₂₆H₂₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	34	26	5	3	0	0
5	B	1	34	26	5	3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	B	1	1	1	0	0
6	A	1	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

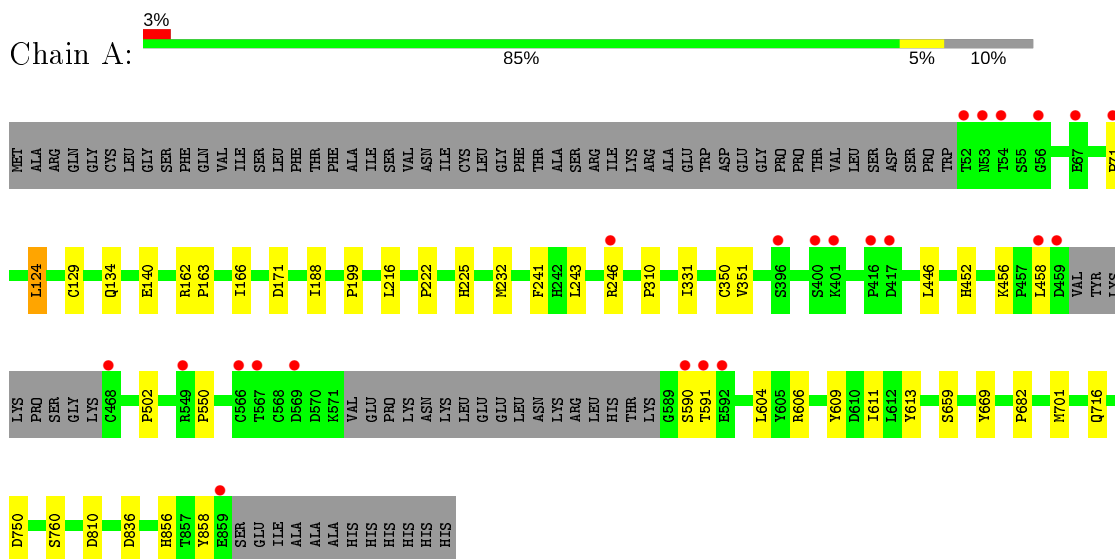
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	40	Total 40	O 40	0	0
8	B	42	Total 42	O 42	0	0

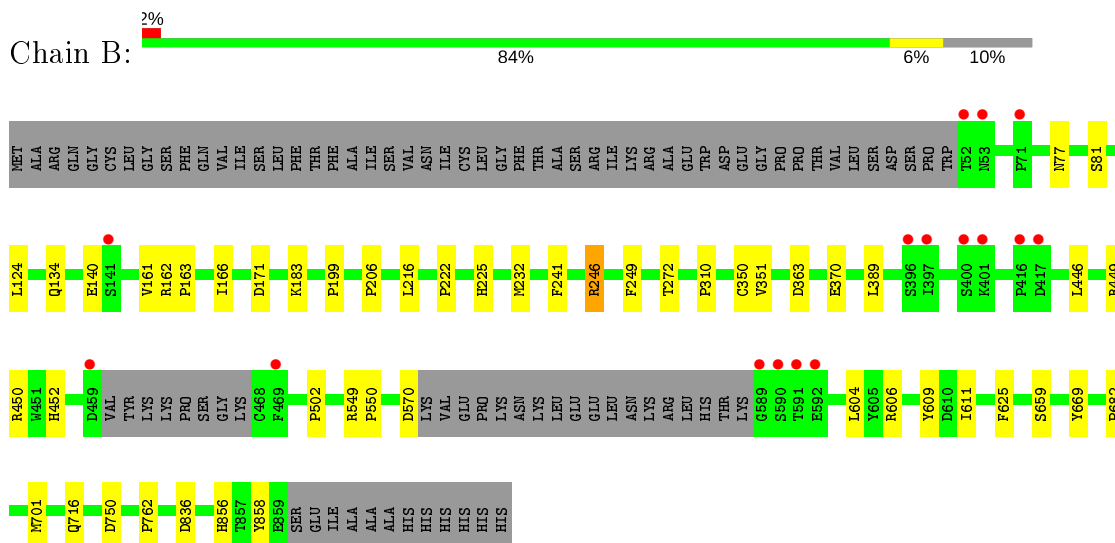
3 Residue-property plots [i](#)

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 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(

1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  22% 78%

MAG1
MAG2
BGA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%

MAG1
MAG2
BGA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.18Å 96.84Å 136.92Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	19.98 – 3.06 19.98 – 3.06	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.98-3.06) 95.0 (19.98-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.04Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.183 , 0.211 0.202 , 0.230	Depositor DCC
R_{free} test set	982 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtrriage
Anisotropy	0.626	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12992	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, 6ZN, MAN

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	0.50	0/6497	0.68	0/8814
1	B	0.51	0/6488	0.69	0/8803
All	All	0.51	0/12985	0.68	0/17617

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 [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	6319	0	6049	20	0
1	B	6310	0	6036	21	0
2	C	105	0	88	0	0
3	D	72	0	61	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	34	0	0	1	0
5	B	34	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	3	0	0	0	0
8	A	40	0	0	0	0
8	B	42	0	0	1	0
All	All	12992	0	12260	40	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 2.

All (40) 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:163:PRO:HB3	1:A:350:CYS:O	1.87	0.75
1:B:77:ASN:OD1	1:B:272:THR:HG21	1.99	0.62
1:A:243:LEU:HD22	5:A:911:6ZN:C7	2.31	0.61
1:A:171:ASP:O	1:A:310:PRO:HD2	2.03	0.58
1:B:171:ASP:O	1:B:310:PRO:HD2	2.05	0.56
1:A:71:PRO:HB3	1:B:549:ARG:HH22	1.72	0.54
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.44	0.53
1:B:222:PRO:HA	1:B:225:HIS:CE1	2.45	0.52
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.93	0.51
1:B:166:ILE:HD12	1:B:351:VAL:HG11	1.93	0.50
1:B:625:PHE:HD1	1:B:762:PRO:HG3	1.76	0.50
1:A:456:LYS:HG3	1:A:458:LEU:HB3	1.94	0.49
1:B:134:GLN:HB3	1:B:140:GLU:HG3	1.95	0.48
1:A:134:GLN:HB3	1:A:140:GLU:HG3	1.95	0.48
1:B:682:PRO:HB3	1:B:716:GLN:HB3	1.96	0.47
1:B:669:TYR:CE2	1:B:701:MET:CE	2.97	0.47
1:A:669:TYR:CE2	1:A:701:MET:CE	2.98	0.46
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.96	0.46
1:B:81:SER:HA	8:B:1038:HOH:O	2.15	0.46
1:B:449:ARG:O	1:B:450:ARG:HB2	2.17	0.45
1:B:604:LEU:HD11	1:B:836:ASP:HB2	1.98	0.45
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.98	0.44
1:A:604:LEU:HD11	1:A:836:ASP:HB2	1.98	0.44
1:B:246:ARG:HA	1:B:249:PHE:HD2	1.84	0.43
1:B:856:HIS:HD2	1:B:858:TYR:CZ	2.36	0.43
1:B:199:PRO:HG2	1:B:502:PRO:HG3	2.00	0.42
1:A:124:LEU:HD12	1:A:129:CYS:SG	2.60	0.42
1:B:550:PRO:HB2	1:B:611:ILE:HG12	2.01	0.42
1:A:856:HIS:HD2	1:A:858:TYR:CZ	2.38	0.42
1:B:206:PRO:HB3	1:B:389:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD11	1:A:331:ILE:HG22	2.02	0.41
1:B:163:PRO:HB3	1:B:350:CYS:O	2.20	0.41
1:A:550:PRO:HB3	1:A:609:TYR:CE2	2.55	0.41
1:B:232:MET:HB2	1:B:241:PHE:HB3	2.01	0.41
1:A:232:MET:HB2	1:A:241:PHE:HB3	2.01	0.41
1:B:550:PRO:HB3	1:B:609:TYR:CE2	2.56	0.41
1:B:669:TYR:CE2	1:B:701:MET:HE1	2.56	0.40
1:A:456:LYS:HE3	1:A:458:LEU:HD22	2.03	0.40
1:A:550:PRO:HB2	1:A:611:ILE:HG12	2.02	0.40
1:A:591:THR:HG21	1:A:613:TYR:HB3	2.04	0.40

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	777/871 (89%)	745 (96%)	31 (4%)	1 (0%)	51 81
1	B	776/871 (89%)	743 (96%)	33 (4%)	0	100 100
All	All	1553/1742 (89%)	1488 (96%)	64 (4%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	SER

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	710/786 (90%)	699 (98%)	11 (2%)	65	83
1	B	709/786 (90%)	695 (98%)	14 (2%)	55	78
All	All	1419/1572 (90%)	1394 (98%)	25 (2%)	59	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	A	162	ARG
1	A	216	LEU
1	A	246	ARG
1	A	446	LEU
1	A	452	HIS
1	A	606	ARG
1	A	659	SER
1	A	750	ASP
1	A	760	SER
1	A	810	ASP
1	B	124	LEU
1	B	161	VAL
1	B	162	ARG
1	B	183	LYS
1	B	216	LEU
1	B	246	ARG
1	B	363	ASP
1	B	370	GLU
1	B	446	LEU
1	B	452	HIS
1	B	570	ASP
1	B	606	ARG
1	B	659	SER
1	B	750	ASP

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

Mol	Chain	Res	Type
1	A	118	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](#)

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	0.73	0	15,15,17	1.23	1 (6%)
2	MAN	C	4	2	11,11,12	0.49	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	0.46	0	15,15,17	0.91	1 (6%)
2	MAN	C	6	2	11,11,12	0.42	0	15,15,17	0.79	1 (6%)
2	MAN	C	7	2	11,11,12	0.37	0	15,15,17	0.89	1 (6%)
2	MAN	C	8	2	11,11,12	0.34	0	15,15,17	0.66	0
2	MAN	C	9	2	11,11,12	0.38	0	15,15,17	0.66	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.39	0	17,19,21	0.98	1 (5%)
3	NAG	D	2	3	14,14,15	0.29	0	17,19,21	0.78	0
3	BMA	D	3	3	11,11,12	0.77	0	15,15,17	1.17	0
3	MAN	D	4	3	11,11,12	0.45	0	15,15,17	0.98	1 (6%)
3	MAN	D	5	3	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
3	MAN	D	6	3	11,11,12	0.40	0	15,15,17	0.84	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	MAN	C1-O5-C5	2.98	116.23	112.19
3	D	1	NAG	O5-C1-C2	-2.96	106.62	111.29
3	D	4	MAN	C1-O5-C5	2.88	116.09	112.19
2	C	5	MAN	C1-O5-C5	2.82	116.02	112.19
3	D	5	MAN	C1-O5-C5	2.80	115.99	112.19
2	C	1	NAG	O5-C1-C2	-2.75	106.95	111.29
2	C	4	MAN	C1-O5-C5	2.73	115.89	112.19
3	D	6	MAN	C1-O5-C5	2.71	115.86	112.19
2	C	3	BMA	C1-C2-C3	-2.58	106.49	109.67
2	C	6	MAN	C1-O5-C5	2.47	115.54	112.19
2	C	9	MAN	C1-C2-C3	2.05	112.19	109.67

There are no chirality outliers.

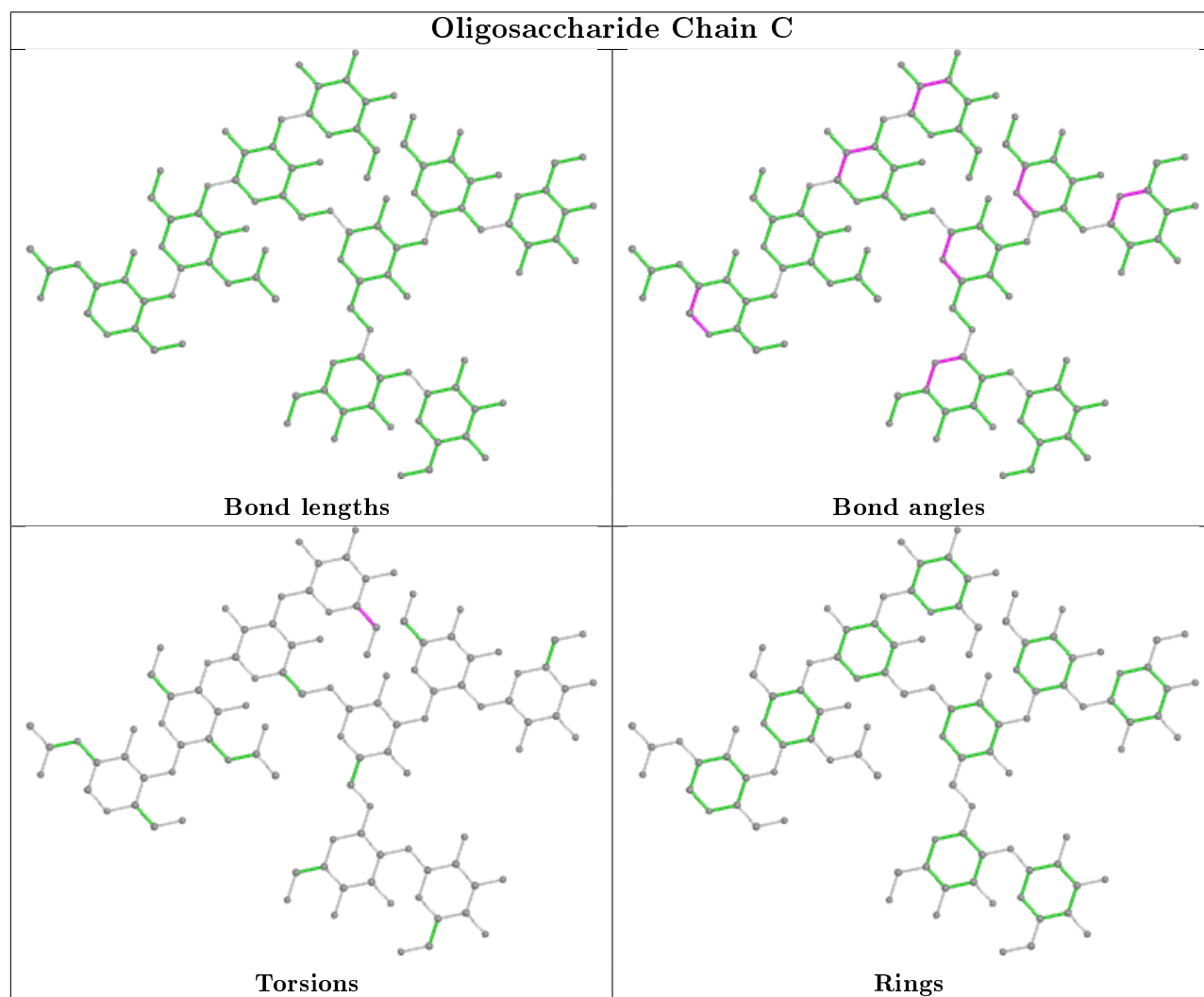
All (2) torsion outliers are listed below:

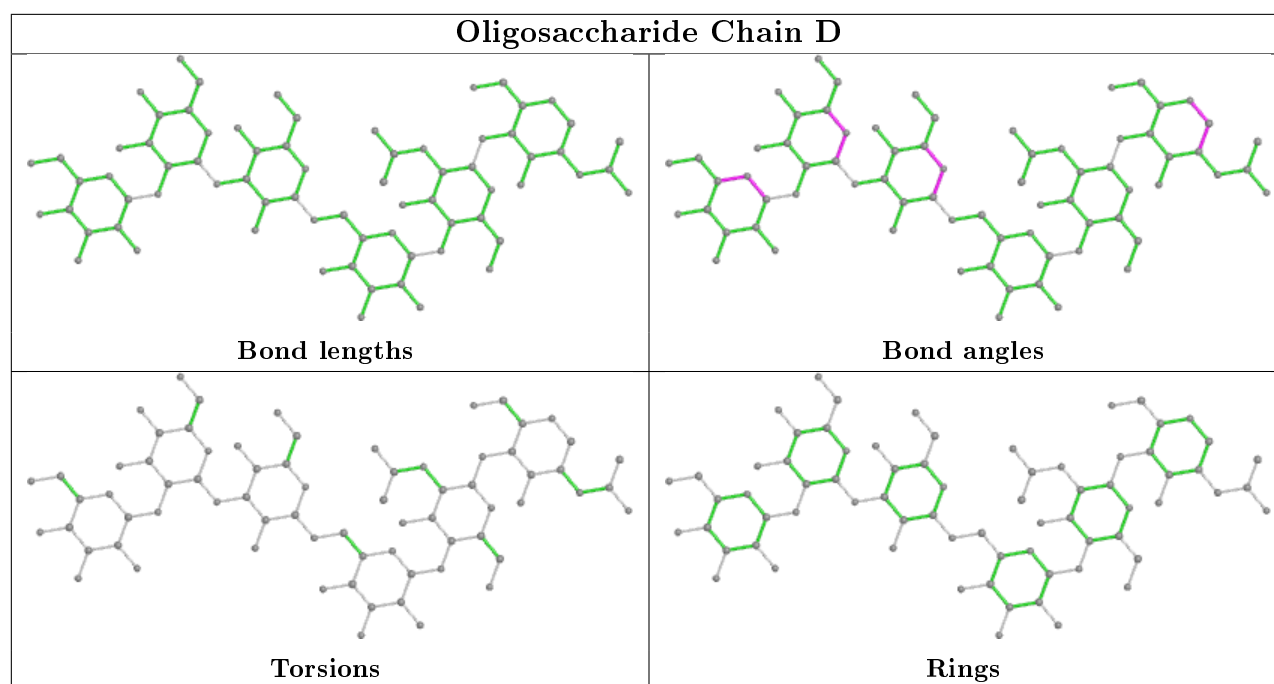
Mol	Chain	Res	Type	Atoms
2	C	9	MAN	C4-C5-C6-O6
2	C	9	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	910	1	14,14,15	0.33	0	17,19,21	0.57	0
4	NAG	B	907	1	14,14,15	0.30	0	17,19,21	0.53	0
5	6ZN	A	911	7	36,39,39	1.47	4 (11%)	44,56,56	2.04	16 (36%)
5	6ZN	B	908	7	36,39,39	1.35	3 (8%)	44,56,56	2.00	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	910	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	6ZN	A	911	7	-	4/13/30/30	0/6/6/6
5	6ZN	B	908	7	-	2/13/30/30	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	911	6ZN	C16-N30	6.10	1.42	1.34
5	B	908	6ZN	C16-N30	5.46	1.41	1.34
5	B	908	6ZN	O32-C17	2.79	1.22	1.19
5	A	911	6ZN	O32-C17	2.78	1.22	1.19
5	A	911	6ZN	C20-C11	-2.26	1.47	1.50
5	A	911	6ZN	C6-C13	-2.18	1.38	1.41
5	B	908	6ZN	C6-C13	-2.16	1.38	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	908	6ZN	C16-N30-C24	-5.84	114.46	124.31
5	B	908	6ZN	N30-C16-N28	4.89	124.52	117.18
5	A	911	6ZN	C21-N31-C26	-4.67	105.89	112.94
5	A	911	6ZN	C16-N30-C24	-4.66	116.45	124.31
5	A	911	6ZN	C26-C25-C18	-3.97	108.01	112.86
5	B	908	6ZN	C11-C20-C24	-3.91	98.98	102.76
5	B	908	6ZN	C10-C19-C24	-3.71	99.18	102.76
5	A	911	6ZN	N30-C16-N28	3.68	122.71	117.18
5	B	908	6ZN	N30-C16-N27	-3.38	110.89	116.65
5	A	911	6ZN	N27-C16-N28	-3.32	123.40	126.55
5	B	908	6ZN	C26-C25-C18	-3.17	108.99	112.86
5	A	911	6ZN	C3-C6-C13	-2.98	117.09	120.84
5	A	911	6ZN	C25-C18-C9	-2.77	115.29	119.13
5	A	911	6ZN	C10-C19-C24	-2.75	100.11	102.76
5	A	911	6ZN	O33-C18-C25	2.65	124.89	120.38
5	B	908	6ZN	C7-C14-C13	-2.63	118.47	121.12
5	A	911	6ZN	C19-C10-C11	2.51	112.28	110.56
5	A	911	6ZN	C1-C4-C10	-2.49	117.17	120.89
5	A	911	6ZN	C3-C9-C7	2.48	122.19	119.23
5	B	908	6ZN	C3-C6-C13	-2.39	117.83	120.84
5	A	911	6ZN	C2-C5-C11	-2.34	117.40	120.89
5	B	908	6ZN	C21-N31-C26	-2.33	109.43	112.94
5	A	911	6ZN	C5-C11-C10	2.29	122.80	120.11
5	A	911	6ZN	C6-C13-C14	2.21	124.42	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	908	6ZN	N27-C16-N28	-2.12	124.54	126.55
5	B	908	6ZN	C1-C4-C10	-2.12	117.73	120.89
5	A	911	6ZN	C7-C14-C13	-2.11	118.99	121.12
5	B	908	6ZN	C25-C18-C9	-2.02	116.33	119.13

There are no chirality outliers.

All (6) torsion outliers are listed below:

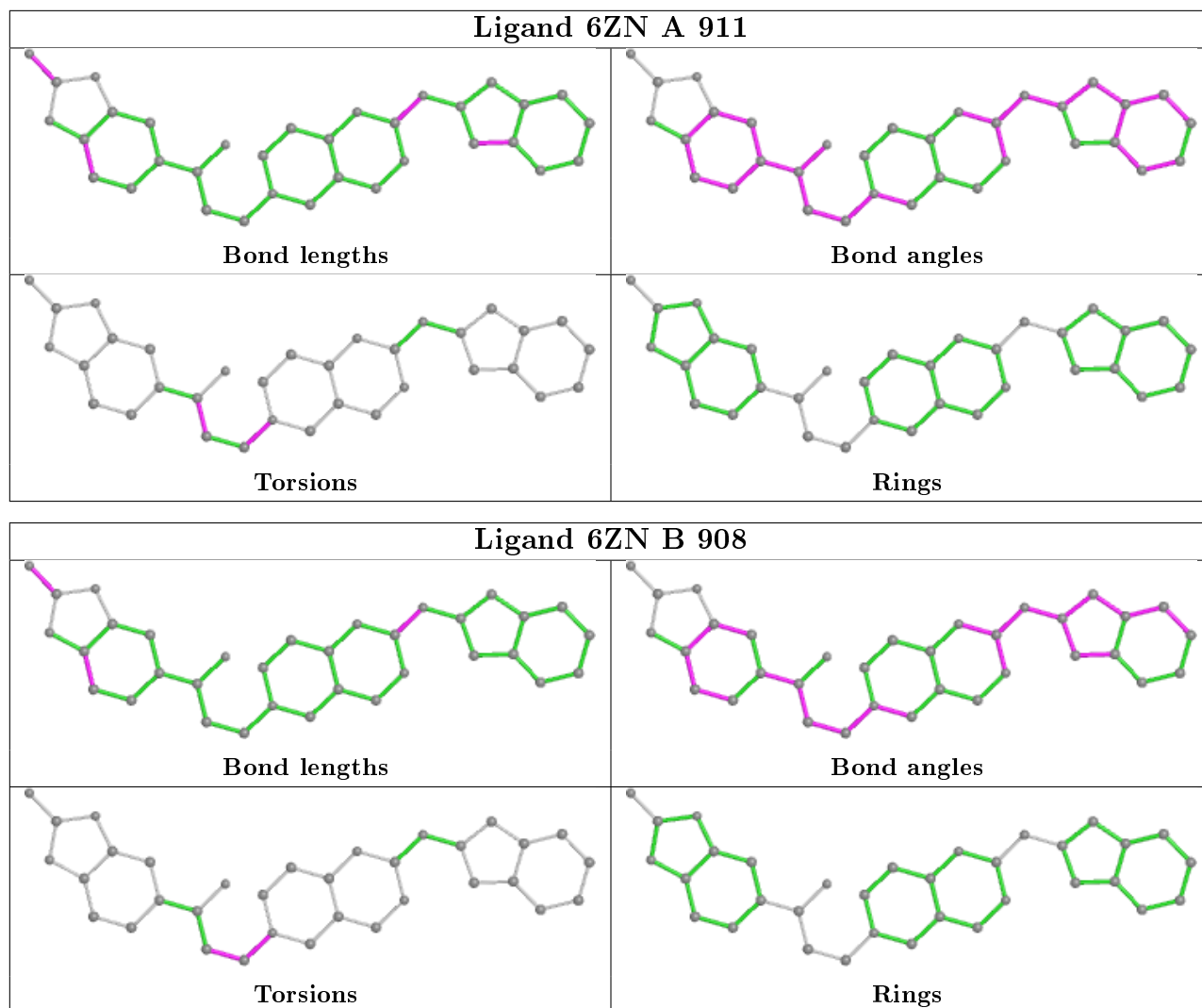
Mol	Chain	Res	Type	Atoms
5	A	911	6ZN	O33-C18-C25-C26
5	A	911	6ZN	C9-C18-C25-C26
5	A	911	6ZN	C25-C26-N31-C21
5	A	911	6ZN	C25-C26-N31-C23
5	B	908	6ZN	C18-C25-C26-N31
5	B	908	6ZN	C25-C26-N31-C21

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	911	6ZN	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 [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	783/871 (89%)	-0.29	23 (2%) 51 26	15, 47, 85, 105	0
1	B	782/871 (89%)	-0.28	16 (2%) 65 41	18, 46, 81, 113	0
All	All	1565/1742 (89%)	-0.28	39 (2%) 57 32	15, 46, 83, 113	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	GLY	5.1
1	B	52	THR	4.8
1	A	400	SER	4.2
1	B	590	SER	4.2
1	A	54	THR	3.9
1	B	396	SER	3.6
1	A	416	PRO	3.2
1	B	417	ASP	3.2
1	A	52	THR	3.0
1	A	459	ASP	3.0
1	A	417	ASP	3.0
1	B	401	LYS	2.9
1	A	71	PRO	2.9
1	A	458	LEU	2.8
1	B	71	PRO	2.7
1	A	566	CYS	2.7
1	A	401	LYS	2.6
1	B	459	ASP	2.6
1	A	67	GLU	2.5
1	B	400	SER	2.5
1	B	591	THR	2.5
1	A	53	ASN	2.4
1	B	416	PRO	2.4
1	A	590	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	246	ARG	2.3
1	A	859	GLU	2.3
1	A	569	ASP	2.3
1	A	396	SER	2.3
1	A	468	CYS	2.3
1	B	592	GLU	2.2
1	A	591	THR	2.2
1	A	56	GLY	2.2
1	A	549	ARG	2.2
1	B	397	ILE	2.1
1	B	53	ASN	2.1
1	B	469	PHE	2.1
1	A	592	GLU	2.0
1	A	567	THR	2.0
1	B	141	SER	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.

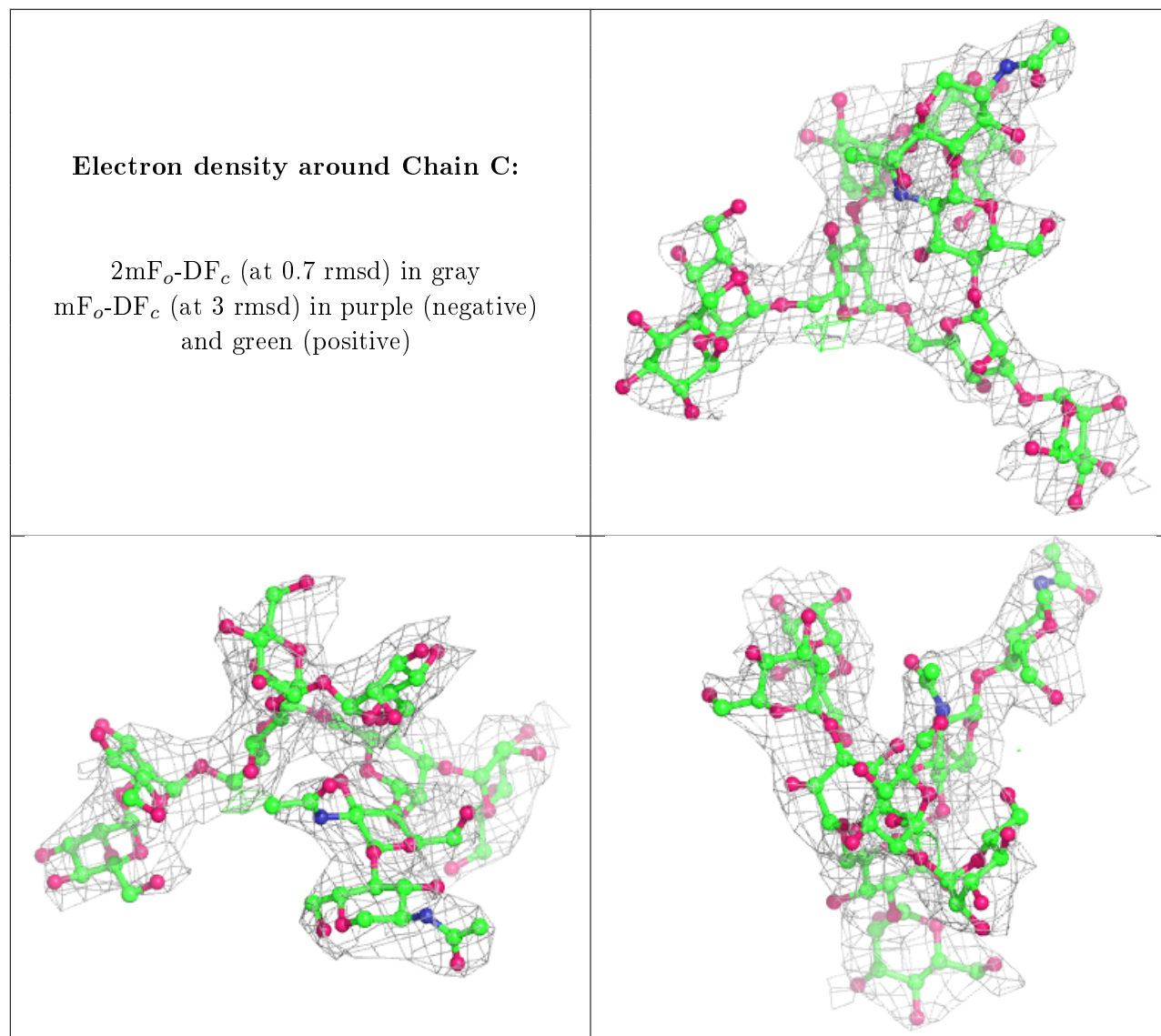
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	3	11/12	0.81	0.36	86,89,90,91	0
2	MAN	C	5	11/12	0.84	0.25	68,73,75,76	0
3	MAN	D	5	11/12	0.85	0.33	96,99,100,101	0
2	MAN	C	8	11/12	0.85	0.31	95,97,100,101	0
3	MAN	D	6	11/12	0.86	0.34	88,91,92,94	0
2	MAN	C	7	11/12	0.86	0.30	88,95,98,98	0
2	MAN	C	9	11/12	0.86	0.42	82,83,84,85	0
3	NAG	D	2	14/15	0.87	0.26	55,64,73,81	0
3	MAN	D	4	11/12	0.91	0.27	81,86,89,93	0
2	BMA	C	3	11/12	0.91	0.33	75,77,78,80	0
2	MAN	C	6	11/12	0.92	0.16	61,65,67,67	0
2	MAN	C	4	11/12	0.92	0.18	68,71,76,81	0
2	NAG	C	2	14/15	0.94	0.25	60,64,70,74	0

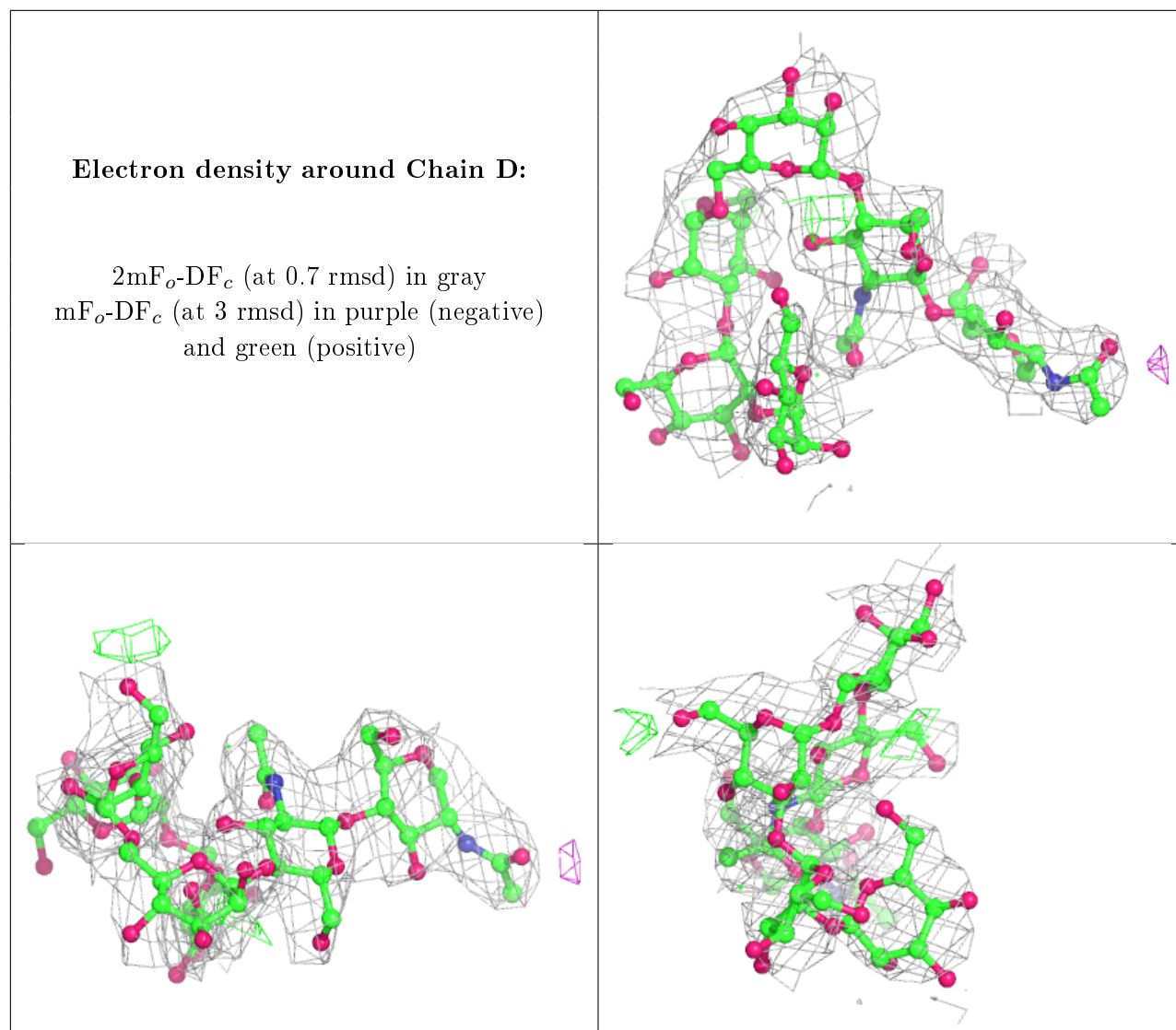
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	1	14/15	0.97	0.14	32,37,44,53	0
2	NAG	C	1	14/15	0.97	0.18	39,46,53,54	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.

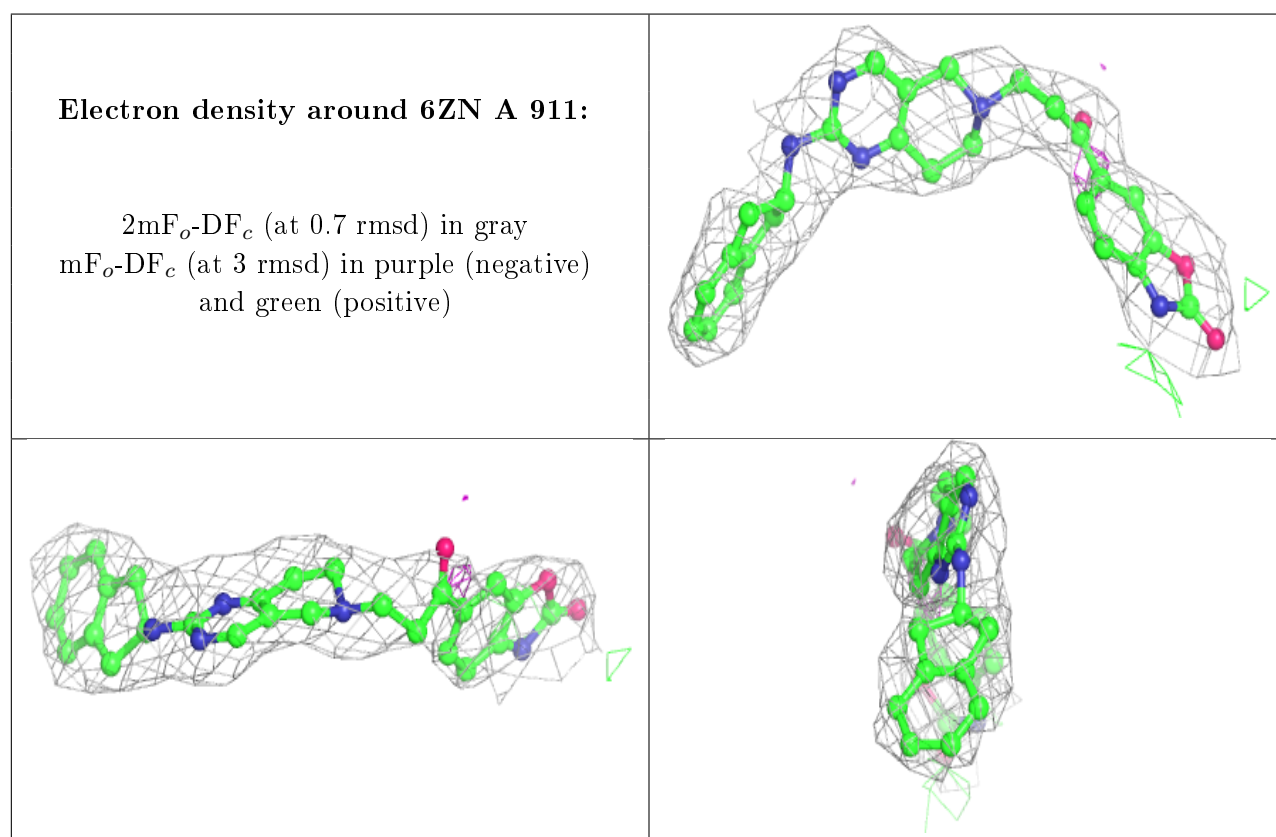
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	907	14/15	0.79	0.34	82,86,90,90	0
4	NAG	A	910	14/15	0.82	0.29	65,71,75,76	0
6	CL	A	912	1/1	0.92	0.11	51,51,51,51	0
5	6ZN	A	911	34/34	0.95	0.17	27,47,61,61	0
7	ZN	B	910	1/1	0.96	0.06	89,89,89,89	0
5	6ZN	B	908	34/34	0.97	0.14	29,36,56,59	0
7	ZN	A	915	1/1	0.98	0.04	72,72,72,72	0

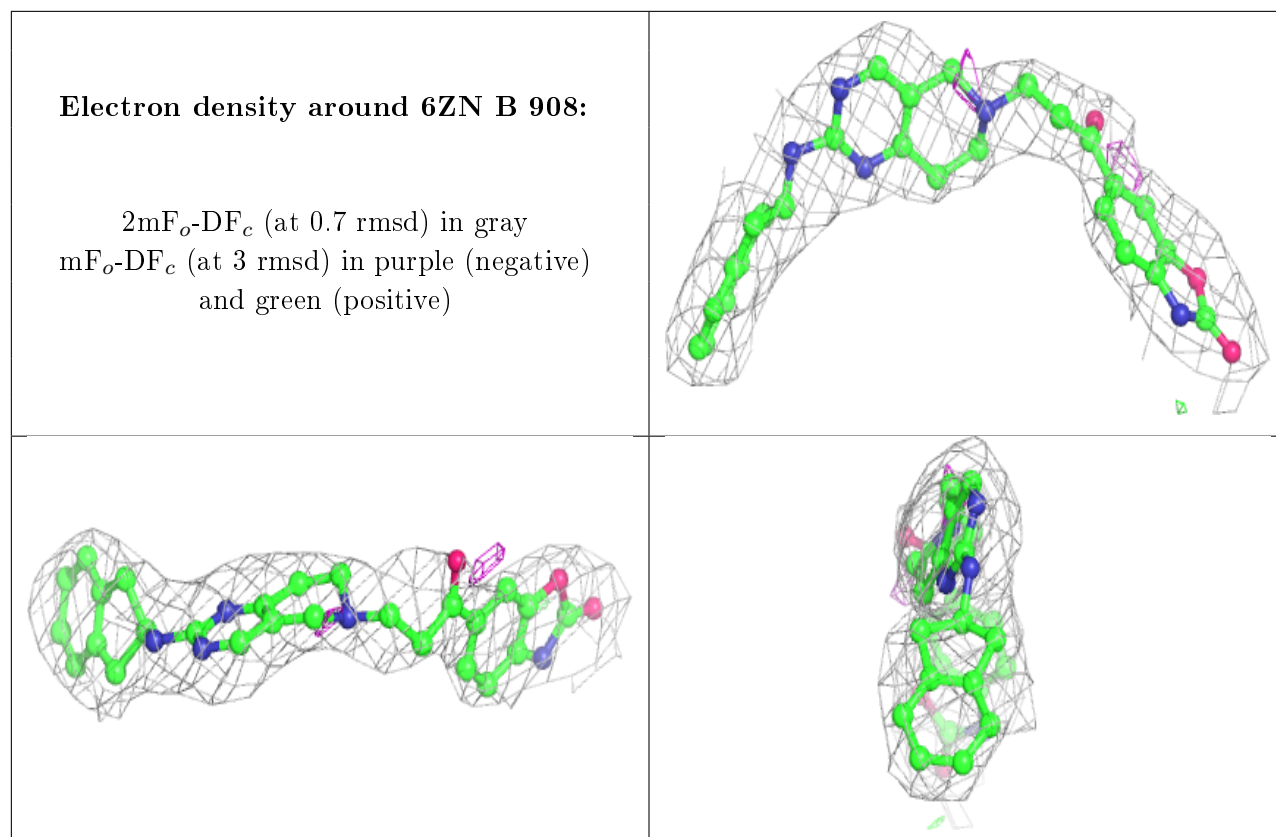
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	A	913	1/1	0.98	0.04	61,61,61,61	1
6	CL	B	912	1/1	0.98	0.12	64,64,64,64	0
7	ZN	B	911	1/1	0.99	0.07	74,74,74,74	0
7	ZN	A	914	1/1	0.99	0.10	30,30,30,30	0
7	ZN	B	909	1/1	1.00	0.08	35,35,35,35	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.