



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2024 – 11:15 AM EDT

PDB ID : 5L0B
Title : Crystal Structure of Autotaxin and Compound 1
Authors : Durbin, J.D.
Deposited on : 2016-07-27
Resolution : 2.41 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

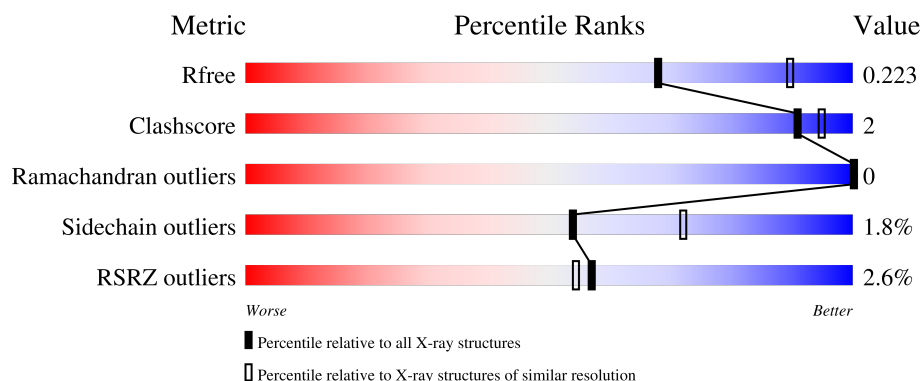
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

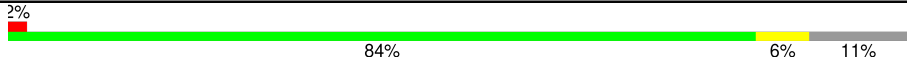



The reported resolution of this entry is 2.41 Å.

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	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	871	 2% 84% 6% 11%
1	B	871	 3% 85% 5% 10%
2	C	9	 33% 67%
3	D	6	 33% 67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13448 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.

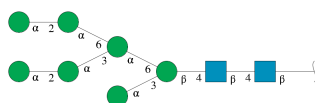
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	0	0
			6293	3987	1084	1173	49			
1	B	781	Total	C	N	O	S	0	0	0
			6307	3995	1086	1177	49			

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

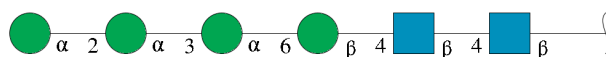
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

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.



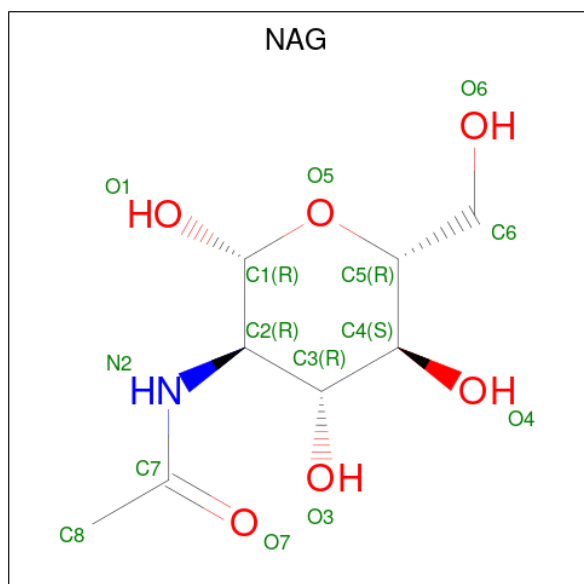
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			

- 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.



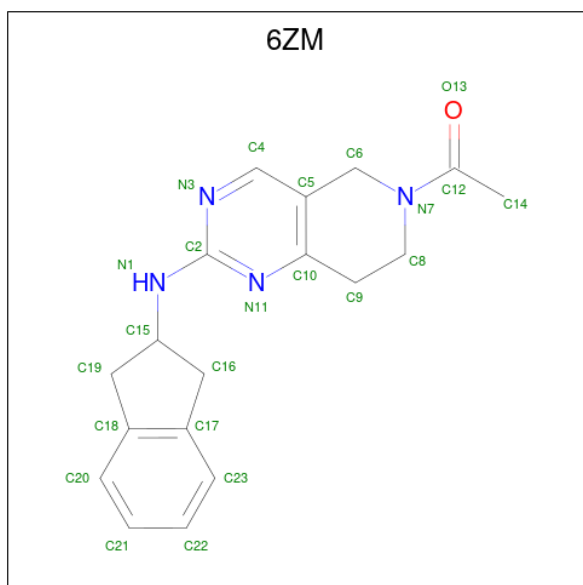
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 5 is 1-{2-[(2,3-dihydro-1H-inden-2-yl)amino]-7,8-dihydropyrido[4,3-d]pyrimidin-6(5H)-yl}ethan-1-one (three-letter code: 6ZM) (formula: C₁₈H₂₀N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	18	4	1		
5	B	1	Total	C	N	O	0	0
			23	18	4	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

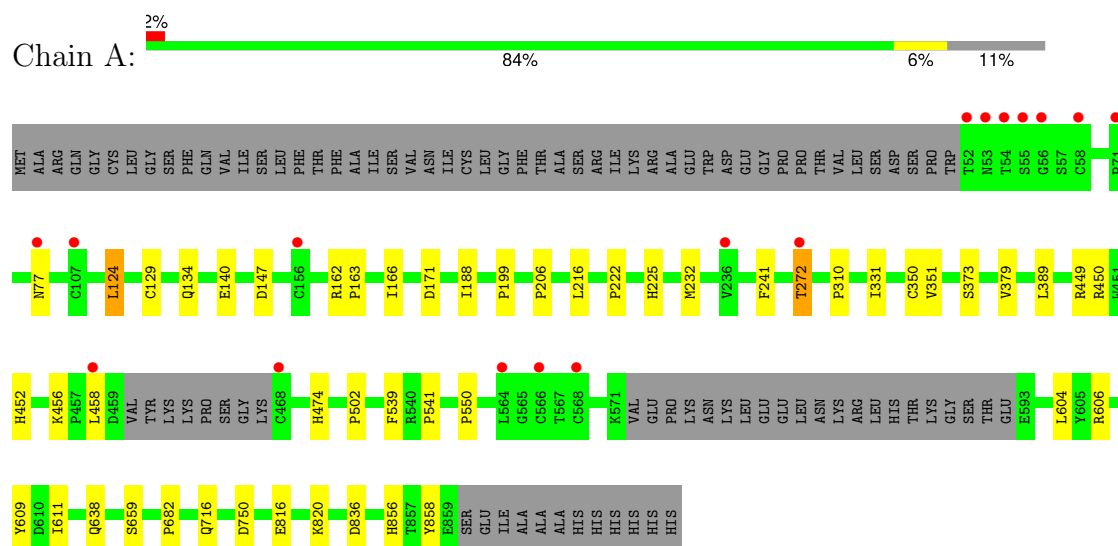
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	341	Total	O	0	0
			341	341		
8	B	248	Total	O	0	0
			248	248		

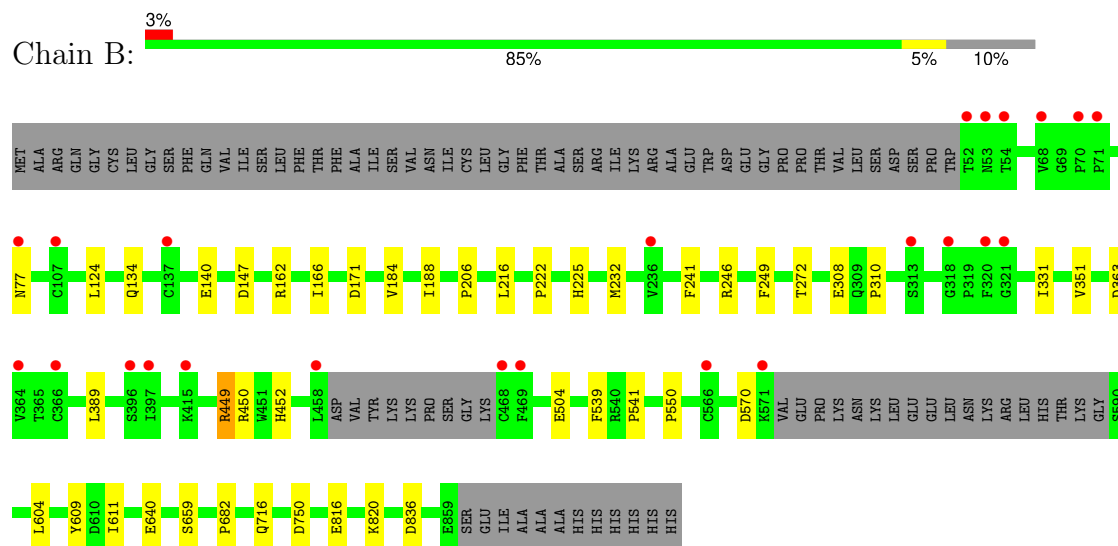
3 Residue-property plots

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:  33% 67%

MAG1	MAG2	BMA3	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	BMA3	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	182.83Å 96.73Å 136.28Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	19.61 – 2.41 19.61 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.61-2.41) 99.7 (19.61-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.176 , 0.209 0.186 , 0.223	Depositor DCC
R_{free} test set	1067 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13448	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: CL, NAG, MAN, BMA, 6ZM, ZN

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	0.51	0/6471	0.67	0/8779
1	B	0.49	0/6485	0.67	0/8798
All	All	0.50	0/12956	0.67	0/17577

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	6293	0	6028	23	0
1	B	6307	0	6042	16	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	23	0	0	0	0
5	B	23	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	1	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	1	0	0	0	0
8	A	341	0	0	1	0
8	B	248	0	0	1	0
All	All	13448	0	12245	39	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 (39) 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	1.92	0.70
1:A:171:ASP:O	1:A:310:PRO:HD2	2.02	0.59
1:B:171:ASP:O	1:B:310:PRO:HD2	2.04	0.57
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.40	0.57
1:B:222:PRO:HA	1:B:225:HIS:CE1	2.41	0.56
1:A:456:LYS:HG3	1:A:458:LEU:HB3	1.91	0.52
1:A:77:ASN:CG	1:A:272:THR:HG21	2.30	0.51
1:B:449:ARG:O	1:B:450:ARG:HB2	2.13	0.49
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.96	0.48
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:A:474:HIS:HE1	8:A:1050:HOH:O	1.95	0.48
1:B:682:PRO:HB3	1:B:716:GLN:HB3	1.96	0.47
1:A:373:SER:HA	1:A:379:VAL:HG11	1.97	0.47
1:B:206:PRO:HB3	1:B:389:LEU:HD22	1.96	0.47
1:B:166:ILE:HD12	1:B:351:VAL:HG11	1.97	0.46
1:A:206:PRO:HB3	1:A:389:LEU:HD22	1.99	0.45
1:B:504:GLU:HB3	8:B:1179:HOH:O	2.17	0.44
1:A:449:ARG:O	1:A:450:ARG:HB2	2.18	0.44
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.99	0.44
1:A:188:ILE:HD11	1:A:331:ILE:HG22	2.00	0.44
1:A:539:PHE:O	1:A:541:PRO:HD3	2.18	0.44
1:B:539:PHE:O	1:B:541:PRO:HD3	2.18	0.43
1:A:124:LEU:HD12	1:A:129:CYS:SG	2.58	0.43
1:B:604:LEU:HD11	1:B:836:ASP:HB2	1.99	0.43
1:A:604:LEU:HD11	1:A:836:ASP:HB2	1.99	0.43
1:B:550:PRO:HB2	1:B:611:ILE:HG12	2.00	0.43
1:A:550:PRO:HB3	1:A:609:TYR:CE2	2.53	0.42
1:B:550:PRO:HB3	1:B:609:TYR:CE2	2.54	0.42
1:B:816:GLU:HG2	1:B:820:LYS:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HA	1:B:249:PHE:HD2	1.85	0.42
1:A:550:PRO:HB2	1:A:611:ILE:HG12	2.00	0.42
1:B:232:MET:HB2	1:B:241:PHE:HB3	2.02	0.41
1:A:232:MET:HB2	1:A:241:PHE:HB3	2.01	0.41
1:B:188:ILE:HD11	1:B:331:ILE:HG22	2.02	0.41
1:A:199:PRO:HG2	1:A:502:PRO:HG3	2.02	0.41
1:A:77:ASN:OD1	1:A:272:THR:HG21	2.21	0.41
1:A:856:HIS:HD2	1:A:858:TYR:CZ	2.39	0.40
1:A:816:GLU:HG2	1:A:820:LYS:HE3	2.03	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	773/871 (89%)	743 (96%)	30 (4%)	0	100	100
1	B	775/871 (89%)	742 (96%)	33 (4%)	0	100	100
All	All	1548/1742 (89%)	1485 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	707/786 (90%)	697 (99%)	10 (1%)	62	79
1	B	709/786 (90%)	694 (98%)	15 (2%)	48	67
All	All	1416/1572 (90%)	1391 (98%)	25 (2%)	54	72

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

Mol	Chain	Res	Type
1	A	124	LEU
1	A	147	ASP
1	A	162	ARG
1	A	216	LEU
1	A	272	THR
1	A	452	HIS
1	A	606	ARG
1	A	638	GLN
1	A	659	SER
1	A	750	ASP
1	B	77	ASN
1	B	124	LEU
1	B	147	ASP
1	B	162	ARG
1	B	184	VAL
1	B	216	LEU
1	B	272	THR
1	B	308	GLU
1	B	363	ASP
1	B	449	ARG
1	B	452	HIS
1	B	570	ASP
1	B	640	GLU
1	B	659	SER
1	B	750	ASP

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 ⓘ

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	2,1	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
2	NAG	C	2	2	14,14,15	0.34	0	17,19,21	0.75	0
2	BMA	C	3	2	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
2	MAN	C	4	2	11,11,12	0.47	0	15,15,17	0.86	1 (6%)
2	MAN	C	5	2	11,11,12	0.47	0	15,15,17	0.69	1 (6%)
2	MAN	C	6	2	11,11,12	0.39	0	15,15,17	0.84	1 (6%)
2	MAN	C	7	2	11,11,12	0.34	0	15,15,17	0.85	1 (6%)
2	MAN	C	8	2	11,11,12	0.29	0	15,15,17	0.52	0
2	MAN	C	9	2	11,11,12	0.36	0	15,15,17	0.58	0
3	NAG	D	1	1,3	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.70	0
3	BMA	D	3	3	11,11,12	0.73	0	15,15,17	0.87	0
3	MAN	D	4	3	11,11,12	0.45	0	15,15,17	0.91	1 (6%)
3	MAN	D	5	3	11,11,12	0.39	0	15,15,17	0.72	1 (6%)
3	MAN	D	6	3	11,11,12	0.38	0	15,15,17	0.88	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/2/19/22	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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	MAN	C1-O5-C5	3.04	116.26	112.19
3	D	6	MAN	C1-O5-C5	2.95	116.14	112.19
3	D	1	NAG	O5-C1-C2	-2.87	106.85	111.29
2	C	6	MAN	C1-O5-C5	2.87	116.03	112.19
3	D	4	MAN	C1-O5-C5	2.82	115.96	112.19
2	C	1	NAG	O5-C1-C2	-2.72	107.08	111.29
2	C	4	MAN	C1-O5-C5	2.56	115.62	112.19
3	D	5	MAN	C1-O5-C5	2.37	115.36	112.19
2	C	5	MAN	C1-O5-C5	2.30	115.27	112.19
2	C	3	BMA	O3-C3-C4	2.29	115.76	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

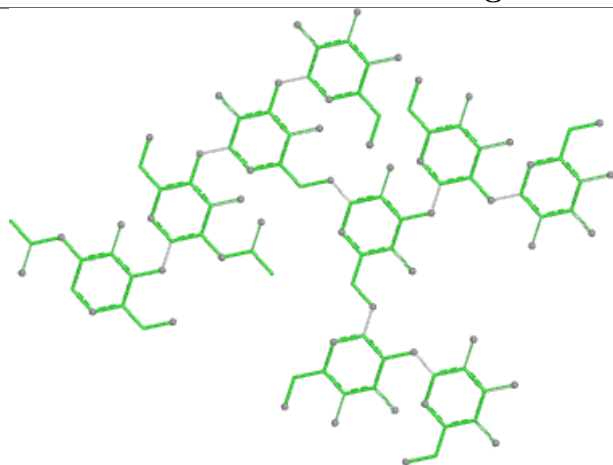
Mol	Chain	Res	Type	Atoms
2	C	9	MAN	C4-C5-C6-O6

There are no ring outliers.

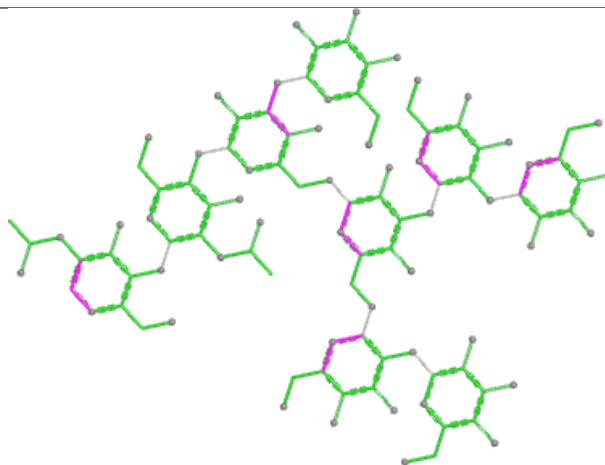
No monomer is involved in short contacts.

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

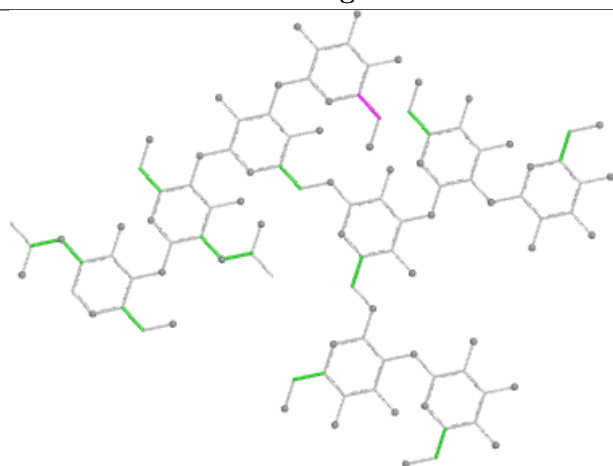
Oligosaccharide Chain C



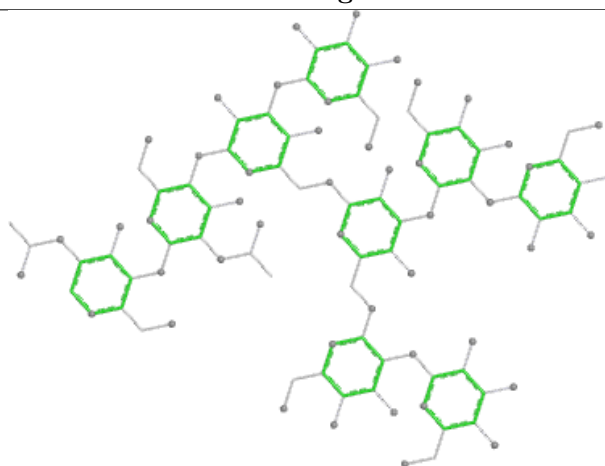
Bond lengths



Bond angles

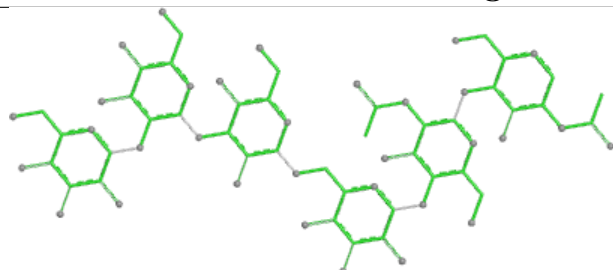


Torsions

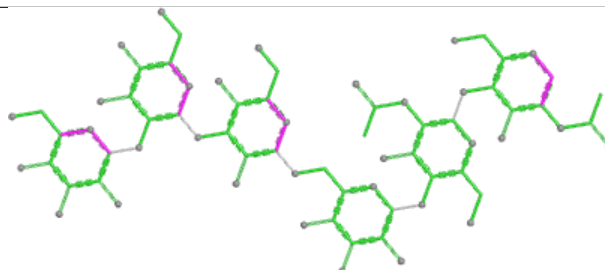


Rings

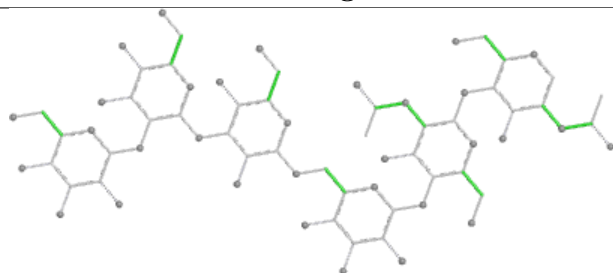
Oligosaccharide Chain D



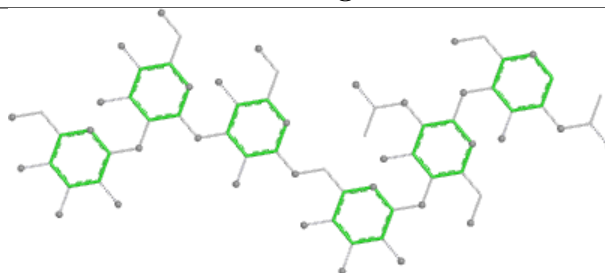
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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
5	6ZM	A	911	-	26,26,26	1.41	1 (3%)	34,37,37	1.90	11 (32%)
4	NAG	B	907	1	14,14,15	0.30	0	17,19,21	0.59	0
5	6ZM	B	908	-	26,26,26	1.36	1 (3%)	34,37,37	2.06	12 (35%)
4	NAG	A	910	1	14,14,15	0.29	0	17,19,21	0.59	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
5	6ZM	A	911	-	-	0/8/25/25	0/4/4/4
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	6ZM	B	908	-	-	4/8/25/25	0/4/4/4
4	NAG	A	910	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	911	6ZM	C2-N1	6.14	1.41	1.34
5	B	908	6ZM	C2-N1	5.54	1.41	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	911	6ZM	O13-C12-N7	4.75	126.57	120.98
5	A	911	6ZM	C2-N1-C15	-4.66	117.07	124.32
5	B	908	6ZM	C14-C12-N7	-4.22	112.90	118.24
5	B	908	6ZM	N1-C2-N11	3.93	123.26	117.09
5	B	908	6ZM	C2-N1-C15	-3.86	118.32	124.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	908	6ZM	O13-C12-N7	3.60	125.22	120.98
5	A	911	6ZM	N1-C2-N11	3.36	122.37	117.09
5	B	908	6ZM	C21-C20-C18	-3.18	116.22	120.88
5	B	908	6ZM	C22-C23-C17	-2.84	116.72	120.88
5	B	908	6ZM	C9-C8-N7	2.76	112.88	110.03
5	B	908	6ZM	C18-C19-C15	-2.68	100.24	102.89
5	B	908	6ZM	N1-C2-N3	-2.68	112.50	116.75
5	A	911	6ZM	N3-C2-N11	-2.68	123.83	126.42
5	A	911	6ZM	C18-C19-C15	-2.61	100.31	102.89
5	A	911	6ZM	C14-C12-N7	-2.46	115.13	118.24
5	A	911	6ZM	C16-C17-C18	2.37	112.09	110.50
5	B	908	6ZM	C17-C16-C15	-2.34	100.58	102.89
5	A	911	6ZM	C21-C20-C18	-2.34	117.45	120.88
5	A	911	6ZM	C17-C16-C15	-2.29	100.63	102.89
5	B	908	6ZM	N3-C2-N11	-2.26	124.23	126.42
5	A	911	6ZM	C9-C8-N7	2.19	112.29	110.03
5	A	911	6ZM	C19-C18-C17	2.15	111.94	110.50
5	B	908	6ZM	C19-C15-N1	-2.07	108.32	112.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

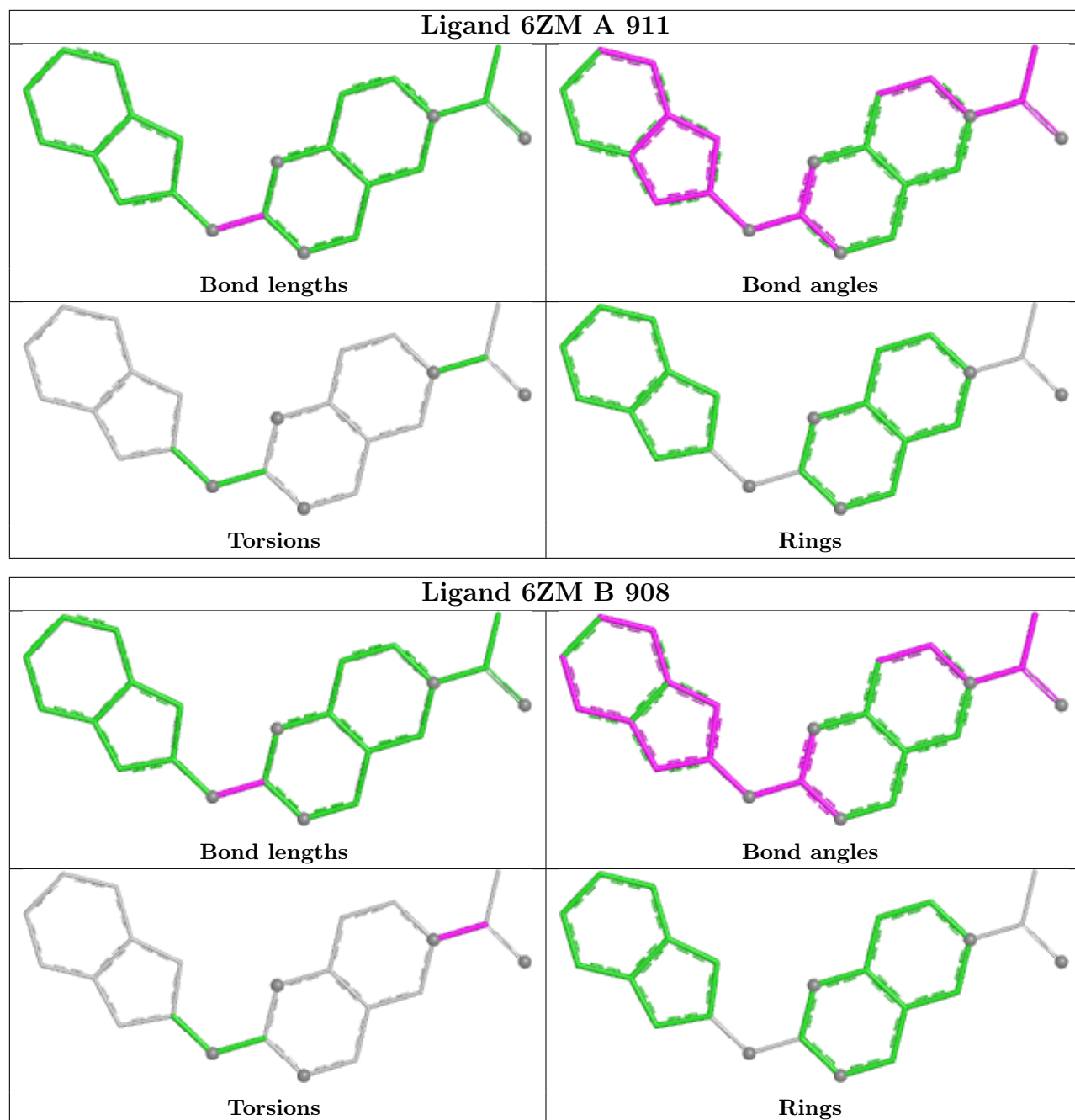
Mol	Chain	Res	Type	Atoms
5	B	908	6ZM	O13-C12-N7-C6
5	B	908	6ZM	C14-C12-N7-C6
5	B	908	6ZM	O13-C12-N7-C8
5	B	908	6ZM	C14-C12-N7-C8

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 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	779/871 (89%)	-0.25	17 (2%) 62 59	19, 37, 71, 102	0
1	B	781/871 (89%)	-0.11	24 (3%) 51 49	21, 42, 79, 106	0
All	All	1560/1742 (89%)	-0.18	41 (2%) 57 54	19, 40, 74, 106	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	LEU	5.0
1	A	54	THR	4.1
1	A	566	CYS	4.0
1	A	56	GLY	3.6
1	A	71	PRO	3.6
1	A	55	SER	3.4
1	A	568	CYS	3.2
1	B	366	CYS	3.1
1	B	396	SER	3.1
1	A	156	CYS	3.0
1	B	469	PHE	2.8
1	B	566	CYS	2.8
1	A	458	LEU	2.8
1	B	318	GLY	2.7
1	B	71	PRO	2.7
1	B	468	CYS	2.7
1	A	52	THR	2.6
1	B	321	GLY	2.6
1	A	236	VAL	2.6
1	B	236	VAL	2.6
1	A	53	ASN	2.6
1	B	137	CYS	2.6
1	B	52	THR	2.5
1	B	54	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	313	SER	2.5
1	A	107	CYS	2.4
1	B	364	VAL	2.4
1	B	107	CYS	2.3
1	B	320	PHE	2.3
1	B	415	LYS	2.2
1	B	571	LYS	2.2
1	B	68	VAL	2.2
1	B	53	ASN	2.2
1	A	58	CYS	2.2
1	A	468	CYS	2.2
1	A	272	THR	2.1
1	B	77	ASN	2.1
1	A	564	LEU	2.1
1	B	70	PRO	2.1
1	A	77	ASN	2.1
1	B	397	ILE	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.

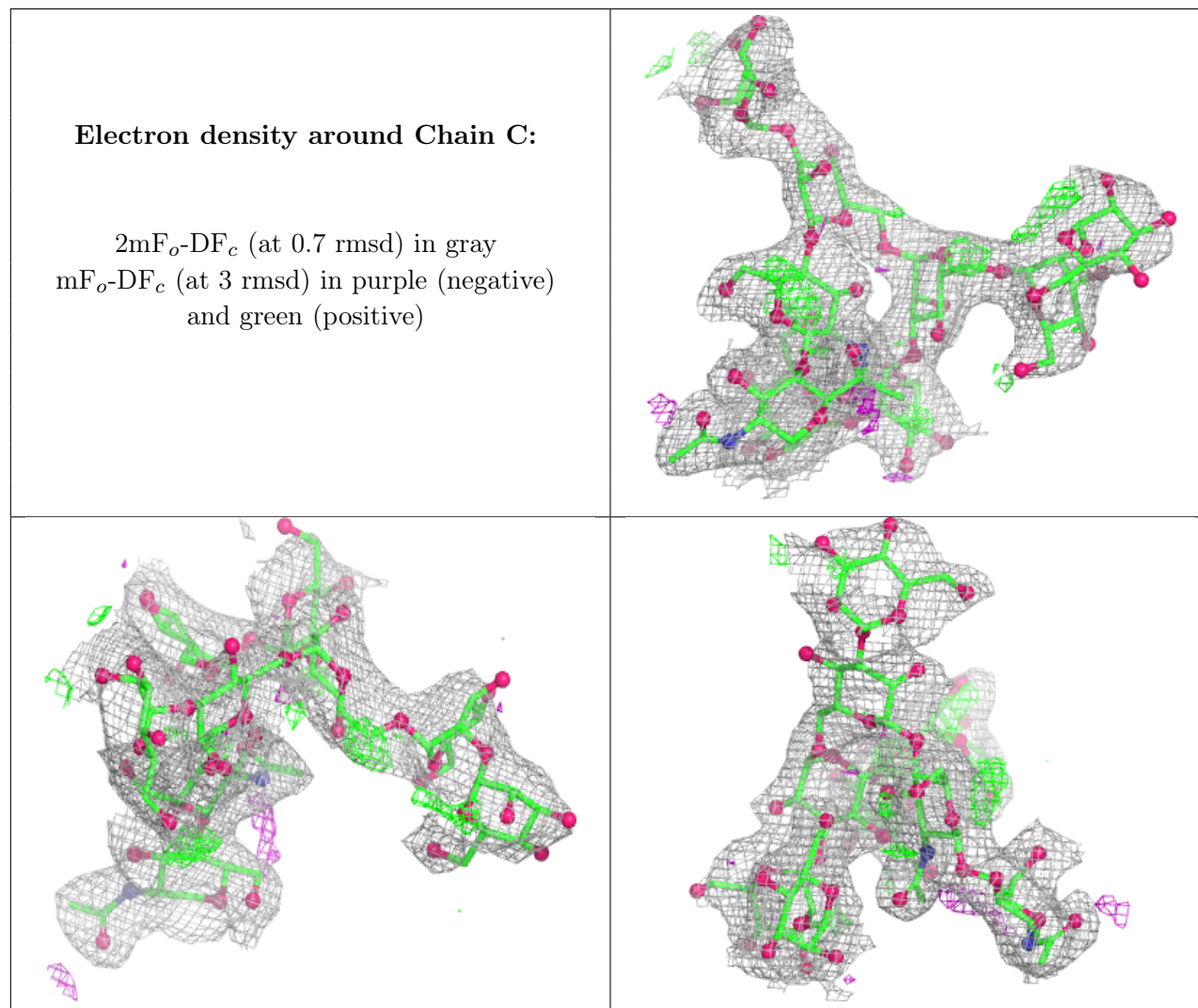
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	9	11/12	0.66	0.11	86,89,90,91	0
3	BMA	D	3	11/12	0.71	0.11	73,77,79,79	0
2	MAN	C	8	11/12	0.75	0.18	91,94,98,100	0
2	MAN	C	7	11/12	0.80	0.16	83,90,93,94	0
3	MAN	D	4	11/12	0.81	0.10	67,75,77,80	0
3	MAN	D	5	11/12	0.81	0.12	78,82,88,91	0
2	BMA	C	3	11/12	0.82	0.14	65,75,79,82	0
2	MAN	C	5	11/12	0.82	0.13	62,67,77,80	0
2	MAN	C	4	11/12	0.87	0.11	57,60,64,72	0
2	NAG	C	2	14/15	0.88	0.10	28,46,56,65	0
3	NAG	D	2	14/15	0.90	0.09	37,53,59,67	0

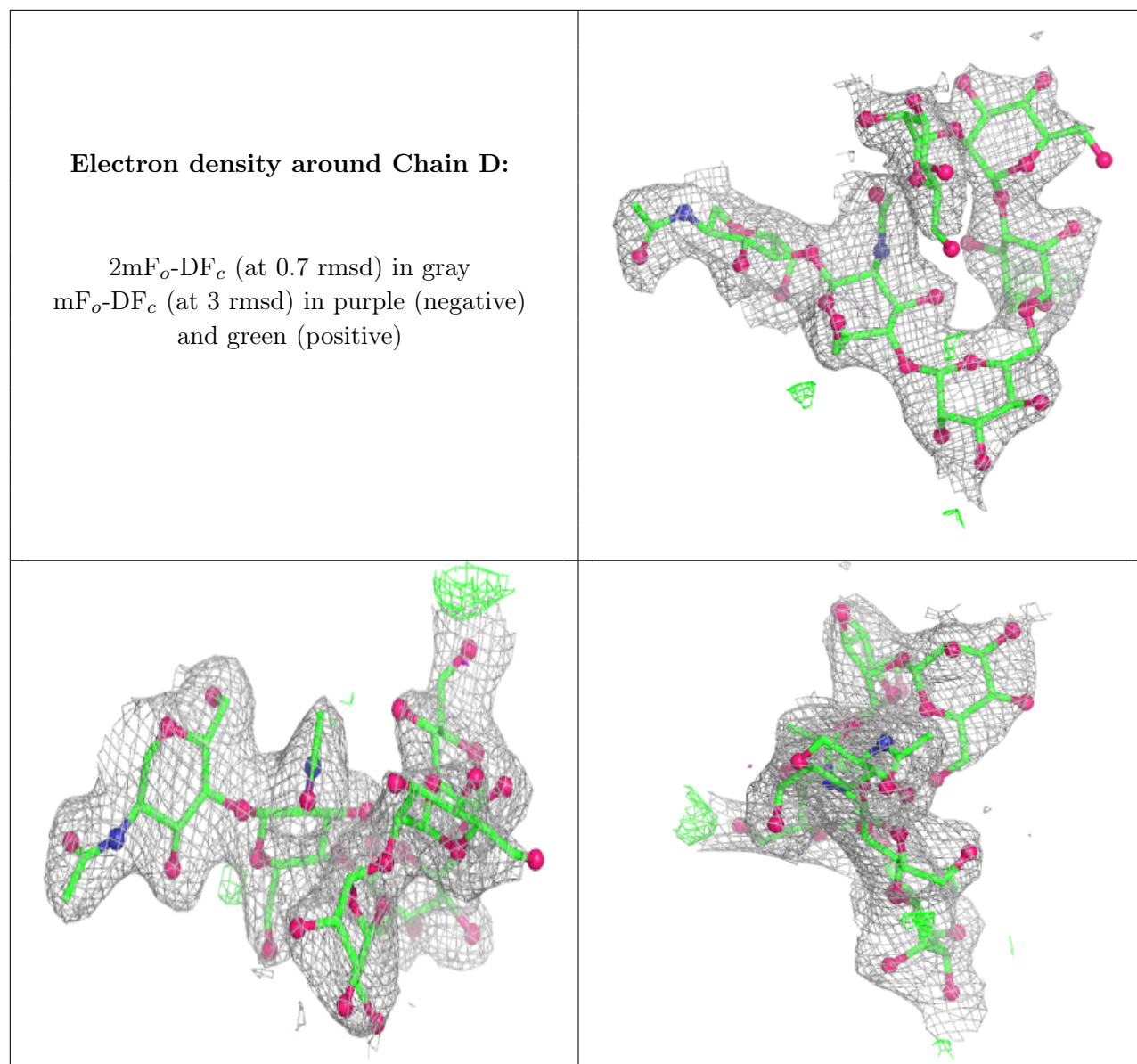
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	D	6	11/12	0.91	0.10	71,74,76,77	0
2	MAN	C	6	11/12	0.92	0.08	48,55,58,58	0
2	NAG	C	1	14/15	0.95	0.07	30,33,39,43	0
3	NAG	D	1	14/15	0.96	0.07	25,35,38,45	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	A	910	14/15	0.78	0.10	45,58,63,64	0
4	NAG	B	907	14/15	0.82	0.10	53,65,70,71	0
5	6ZM	B	908	23/23	0.93	0.08	29,44,65,66	0
5	6ZM	A	911	23/23	0.95	0.06	20,33,44,50	0
7	CL	B	912	1/1	0.96	0.08	58,58,58,58	0

Continued on next page...

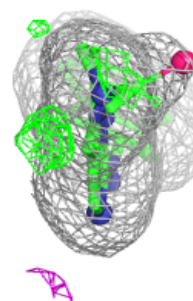
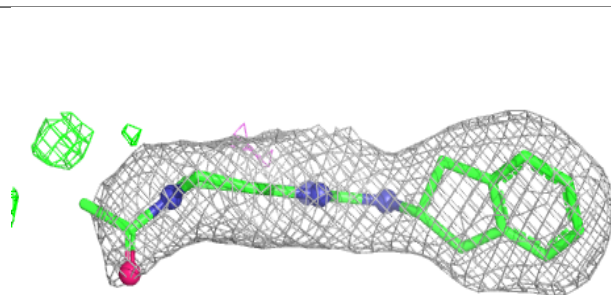
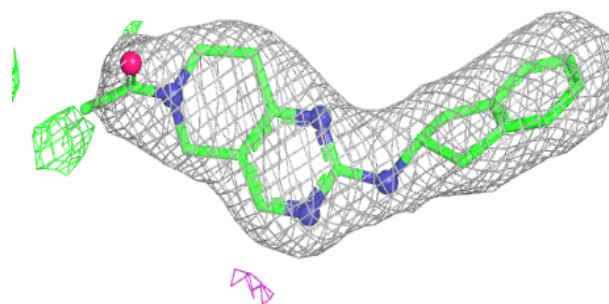
Continued from previous page...

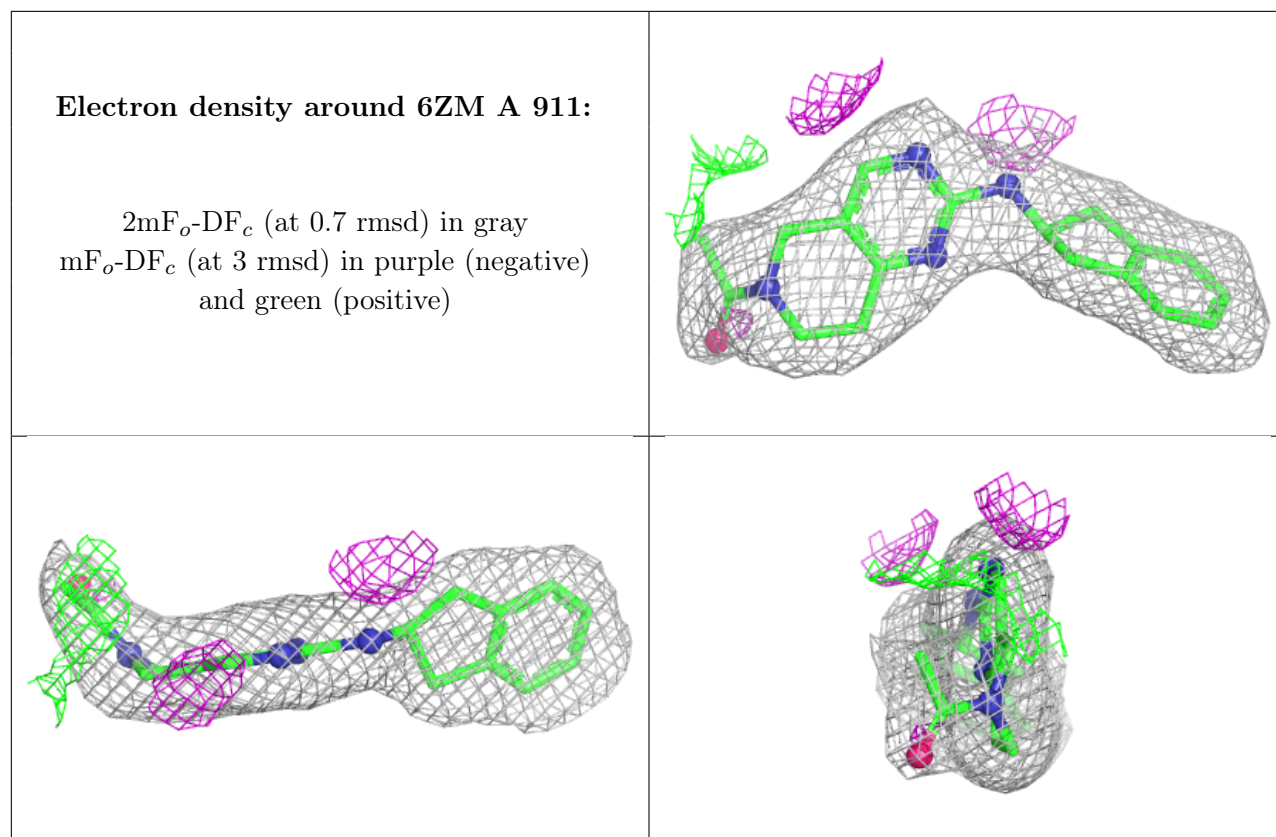
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CL	A	915	1/1	0.98	0.04	44,44,44,44	0
6	ZN	B	910	1/1	0.98	0.05	55,55,55,55	0
6	ZN	B	911	1/1	0.99	0.05	52,52,52,52	0
6	ZN	B	909	1/1	0.99	0.03	59,59,59,59	0
6	ZN	A	913	1/1	0.99	0.03	32,32,32,32	0
6	ZN	A	914	1/1	1.00	0.04	53,53,53,53	0
6	ZN	A	912	1/1	1.00	0.02	29,29,29,29	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 6ZM B 908:

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.