wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 12:28 AM EDT

PDB ID	:	4MN8
Title	:	Crystal structure of flg22 in complex with the FLS2 and BAK1 ectodomains
Authors	:	Chai, J.; Sun, Y.; Han, Z.
Deposited on	:	2013-09-10
Resolution	:	3.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

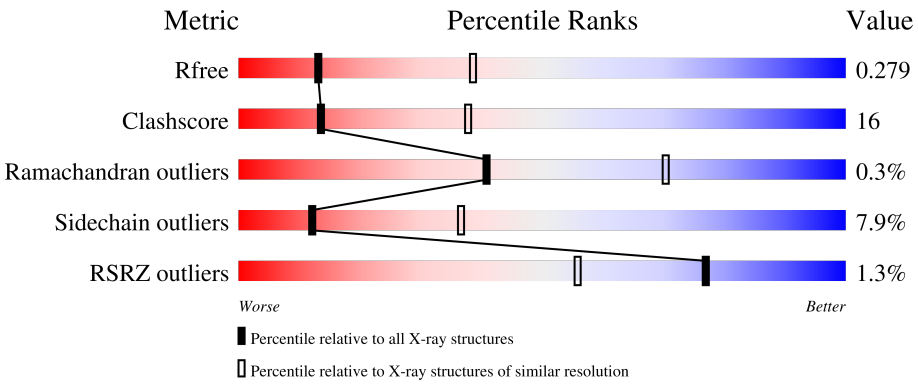
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 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 <=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	782	69% 24% • •
2	B	226	4% 55% 18% • 23%
3	C	22	5% 91% 5% 5%
4	D	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7487 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 LRR receptor-like serine/threonine-protein kinase FLS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	5813	3684	969	1138	22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	801	HIS	-	expression tag	UNP Q9FL28
A	802	HIS	-	expression tag	UNP Q9FL28
A	803	HIS	-	expression tag	UNP Q9FL28
A	804	HIS	-	expression tag	UNP Q9FL28
A	805	HIS	-	expression tag	UNP Q9FL28
A	806	HIS	-	expression tag	UNP Q9FL28

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	1287	808	223	253	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	HIS	-	expression tag	UNP Q94F62
B	222	HIS	-	expression tag	UNP Q94F62
B	223	HIS	-	expression tag	UNP Q94F62
B	224	HIS	-	expression tag	UNP Q94F62
B	225	HIS	-	expression tag	UNP Q94F62
B	226	HIS	-	expression tag	UNP Q94F62

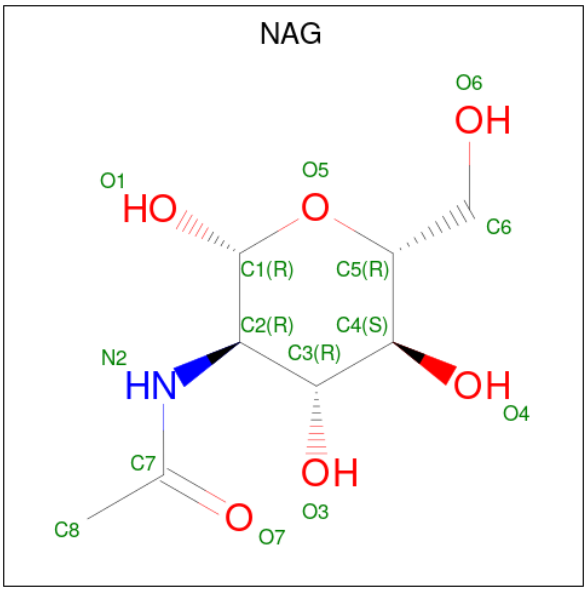
- Molecule 3 is a protein called flg22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	21	153	90	31	32	0	0	0

- Molecule 4 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			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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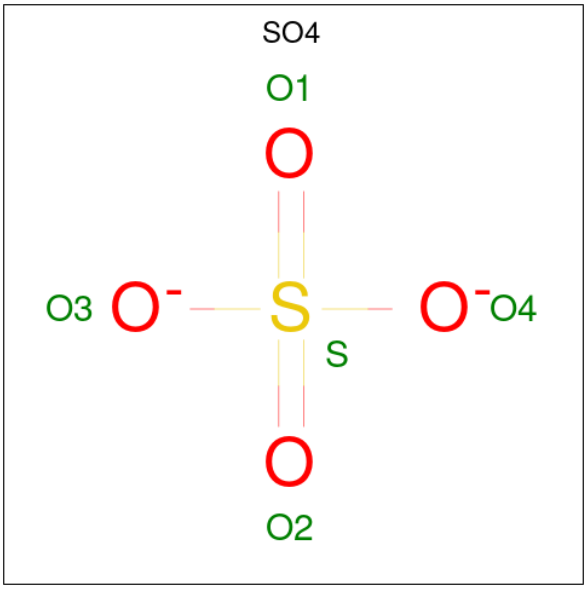
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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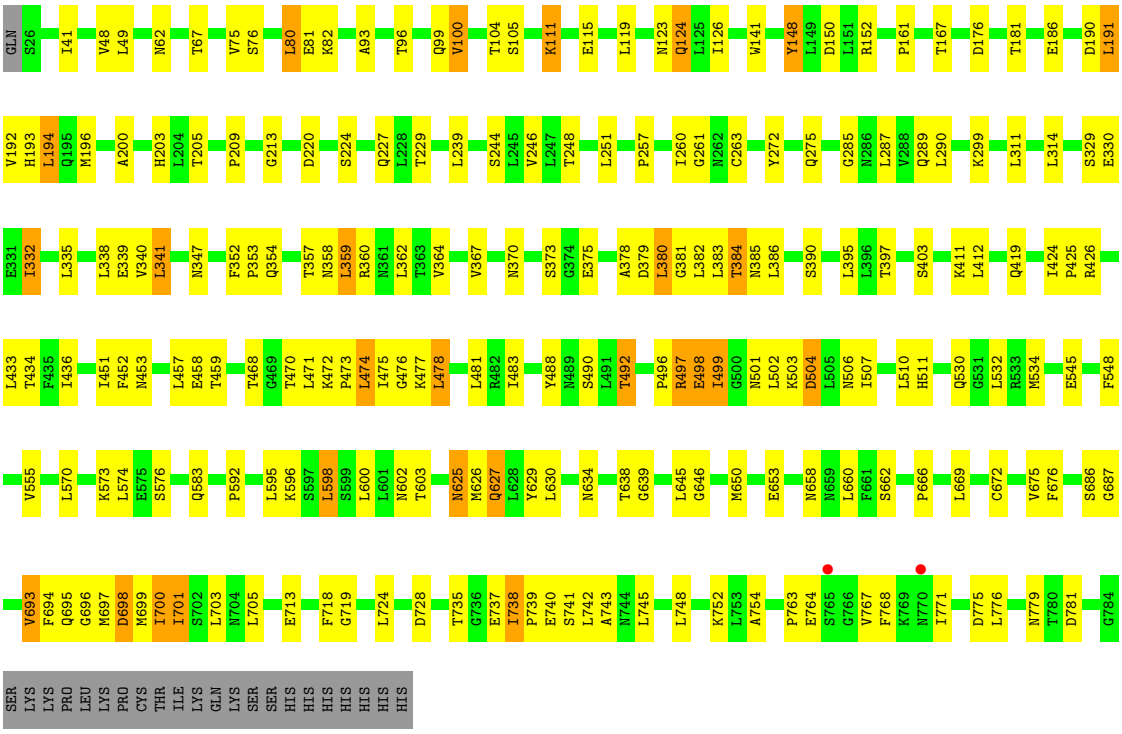
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	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.

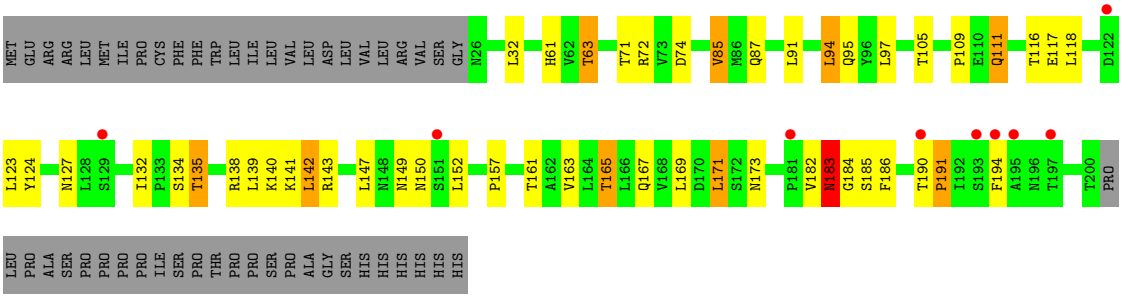
• Molecule 1: LRR receptor-like serine/threonine-protein kinase FLS2

Chain A:



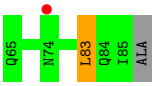
• Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1

Chain B:



• Molecule 3: flg22

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.86Å 113.68Å 164.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.06 29.96 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.96-3.06) 98.6 (29.96-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.224 , 0.275 0.231 , 0.279	Depositor DCC
R_{free} test set	1932 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7487	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, SO4

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	0.32	0/5910	0.55	0/8025
2	B	0.26	0/1307	0.56	0/1789
3	C	0.24	0/152	0.44	0/202
All	All	0.31	0/7369	0.55	0/10016

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	PRO	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	5813	0	5869	211	0
2	B	1287	0	1243	30	0
3	C	153	0	155	1	0
4	D	28	0	25	1	0
5	A	126	0	117	1	0
6	A	60	0	0	2	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
All	All	7487	0	7409	238	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 16.

The worst 5 of 238 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:474:LEU:H	1:A:474:LEU:CD1	1.54	1.20
1:A:738:ILE:HD13	1:A:738:ILE:C	1.56	1.17
1:A:474:LEU:N	1:A:474:LEU:HD12	1.52	1.17
1:A:383:LEU:O	1:A:384:THR:HG23	1.45	1.16
1:A:694:PHE:CD1	1:A:718:PHE:HE1	1.63	1.13

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	757/782 (97%)	707 (93%)	50 (7%)	0	100 100
2	B	173/226 (76%)	153 (88%)	17 (10%)	3 (2%)	9 32
3	C	19/22 (86%)	19 (100%)	0	0	100 100
All	All	949/1030 (92%)	879 (93%)	67 (7%)	3 (0%)	41 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	191	PRO
2	B	183	ASN
2	B	190	THR

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	676/699 (97%)	623 (92%)	53 (8%)	12	37
2	B	139/203 (68%)	127 (91%)	12 (9%)	10	33
3	C	16/16 (100%)	15 (94%)	1 (6%)	18	45
All	All	831/918 (90%)	765 (92%)	66 (8%)	12	36

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	116	THR
2	B	135	THR
3	C	83	LEU
1	A	451	ILE
1	A	390	SER

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

Mol	Chain	Res	Type
1	A	506	ASN

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	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.64	0	17,19,21	0.66	0
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	0.78	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	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

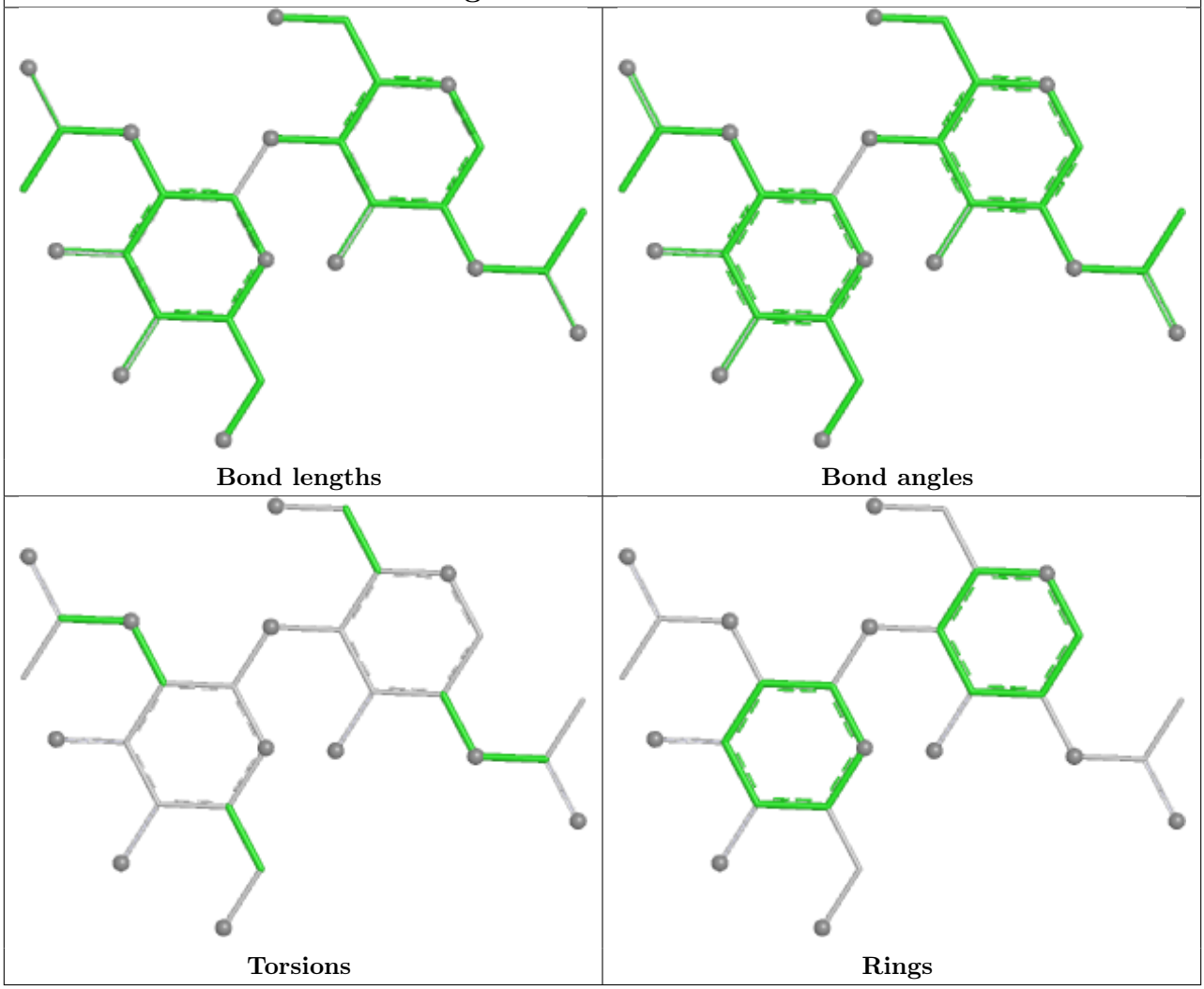
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

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

Oligosaccharide Chain D



5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	905	1	14,14,15	0.60	0	17,19,21	0.96	0
6	SO4	A	912	-	4,4,4	0.24	0	6,6,6	0.11	0
5	NAG	A	903	1	14,14,15	0.51	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	A	922	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	920	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.09	0
5	NAG	A	923	-	14,14,15	0.67	0	19,19,21	1.21	3 (15%)
6	SO4	A	915	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	917	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	921	-	4,4,4	0.23	0	6,6,6	0.08	0
5	NAG	A	910	1	14,14,15	0.57	0	17,19,21	1.05	2 (11%)
6	SO4	A	913	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	A	901	1	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	A	919	-	4,4,4	0.22	0	6,6,6	0.12	0
6	SO4	A	918	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	914	-	4,4,4	0.24	0	6,6,6	0.06	0
5	NAG	A	906	1	14,14,15	0.51	0	17,19,21	0.76	0
5	NAG	A	902	1	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
6	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.08	0
5	NAG	A	904	1	14,14,15	0.41	0	17,19,21	1.92	3 (17%)
6	SO4	A	916	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	911	-	4,4,4	0.24	0	6,6,6	0.12	0
5	NAG	A	909	-	14,14,15	0.49	0	17,19,21	0.73	0
6	SO4	C	101	-	4,4,4	0.24	0	6,6,6	0.06	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	NAG	A	905	1	-	3/6/23/26	0/1/1/1
5	NAG	A	902	1	-	5/6/23/26	0/1/1/1
5	NAG	A	901	1	-	3/6/23/26	0/1/1/1
5	NAG	A	923	-	-	4/6/22/26	0/1/1/1
5	NAG	A	903	1	-	2/6/23/26	0/1/1/1
5	NAG	A	910	1	-	2/6/23/26	0/1/1/1
5	NAG	A	904	1	-	4/6/23/26	0/1/1/1
5	NAG	A	909	-	-	2/6/23/26	0/1/1/1
5	NAG	A	906	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	904	NAG	C1-O5-C5	6.49	120.88	112.19
5	A	901	NAG	C1-O5-C5	3.75	117.21	112.19
5	A	923	NAG	C3-C4-C5	2.60	115.58	111.19
5	A	923	NAG	O5-C5-C4	2.51	113.97	110.14
5	A	910	NAG	C1-O5-C5	2.50	115.53	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	NAG	C3-C2-N2-C7
5	A	901	NAG	C8-C7-N2-C2
5	A	901	NAG	O7-C7-N2-C2
5	A	902	NAG	C3-C2-N2-C7
5	A	902	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	920	SO4	1	0
5	A	904	NAG	1	0
6	A	911	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	759/782 (97%)	-0.45	2 (0%)	94	85	53, 87, 141, 187	0
2	B	175/226 (77%)	0.05	9 (5%)	28	12	66, 120, 195, 239	0
3	C	21/22 (95%)	0.30	1 (4%)	30	13	77, 108, 143, 166	0
All	All	955/1030 (92%)	-0.34	12 (1%)	77	56	53, 91, 154, 239	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	PRO	4.5
2	B	190	THR	4.0
2	B	197	THR	4.0
1	A	765	SER	3.0
2	B	194	PHE	3.0

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.

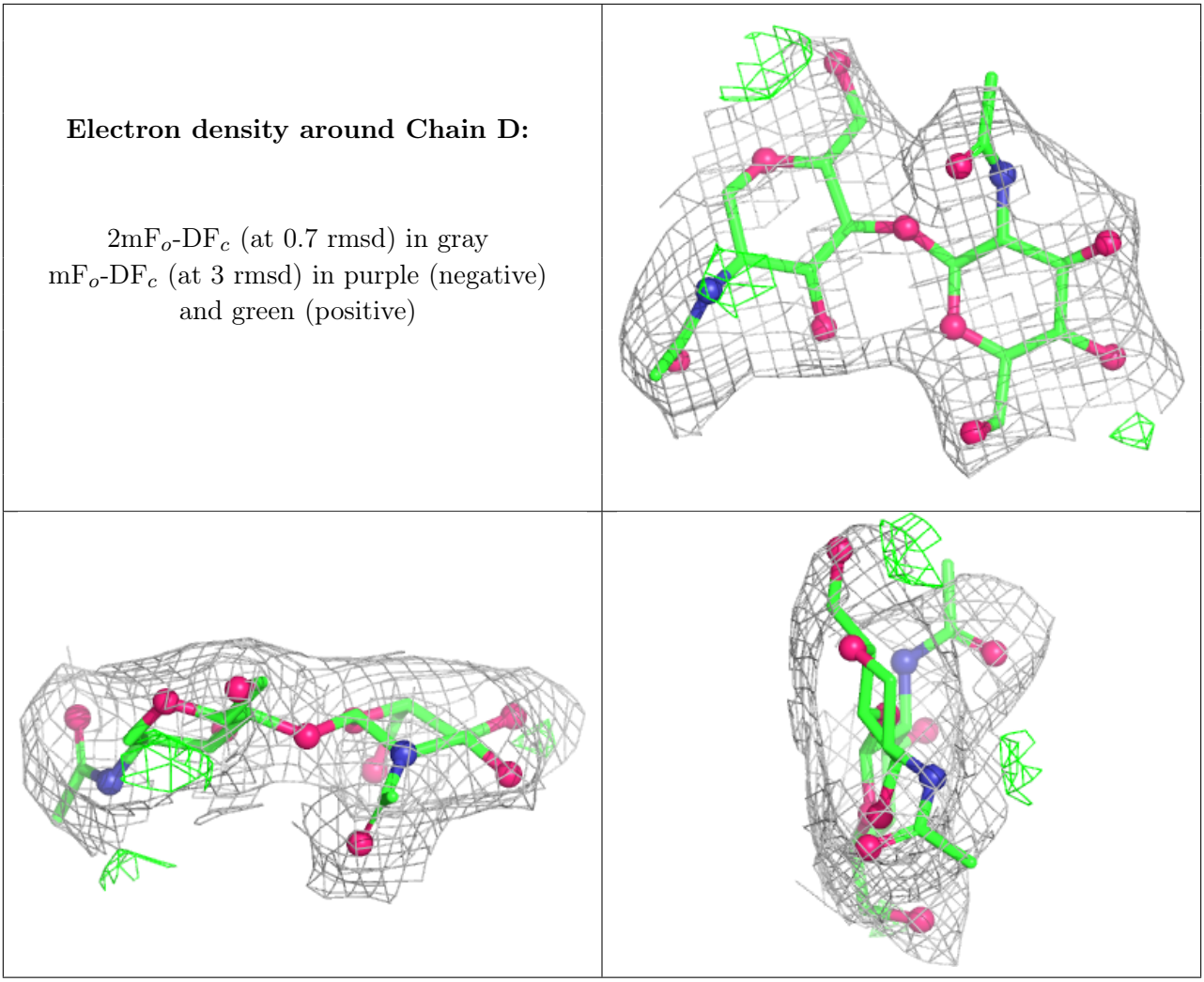
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	2	14/15	0.90	0.21	100,119,125,126	0
4	NAG	D	1	14/15	0.96	0.13	65,72,91,96	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	918	5/5	0.76	0.31	170,170,172,178	0
6	SO4	A	922	5/5	0.76	0.18	196,202,207,212	0
5	NAG	A	910	14/15	0.82	0.17	91,115,135,141	0
6	SO4	A	919	5/5	0.84	0.26	120,126,135,148	0
5	NAG	A	909	14/15	0.84	0.26	128,135,153,158	0
6	SO4	A	917	5/5	0.85	0.27	175,178,179,183	0
5	NAG	A	923	14/15	0.85	0.16	75,121,129,134	0
6	SO4	B	303	5/5	0.85	0.49	159,164,165,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	B	302	5/5	0.86	0.24	133,153,160,160	0
5	NAG	A	906	14/15	0.86	0.44	20,20,20,20	0
5	NAG	A	904	14/15	0.87	0.24	73,90,104,111	0
5	NAG	A	902	14/15	0.88	0.25	111,141,149,157	0
5	NAG	A	901	14/15	0.88	0.18	125,136,156,159	0
6	SO4	B	301	5/5	0.89	0.25	132,135,139,144	0
5	NAG	A	905	14/15	0.90	0.17	101,111,125,130	0
5	NAG	A	903	14/15	0.91	0.25	110,122,136,138	0
6	SO4	A	921	5/5	0.91	0.18	173,174,175,179	0
6	SO4	A	913	5/5	0.92	0.18	166,172,174,178	0
6	SO4	A	916	5/5	0.93	0.49	132,138,141,145	0
6	SO4	A	911	5/5	0.94	0.28	102,112,115,119	0
6	SO4	A	912	5/5	0.94	0.13	94,115,126,139	0
6	SO4	A	915	5/5	0.95	0.27	111,121,123,125	0
6	SO4	C	101	5/5	0.95	0.17	124,131,133,143	0
6	SO4	A	914	5/5	0.96	0.15	128,140,141,144	0
6	SO4	A	920	5/5	0.97	0.12	146,152,158,160	0

6.5 Other polymers (i)

There are no such residues in this entry.