wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 08:01 AM EDT

PDB ID	:	6WDQ
Title	:	IL23/IL23R/IL12Rb1 signaling complex
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Deposited on	:	2020-04-01
Resolution	:	3.40 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:

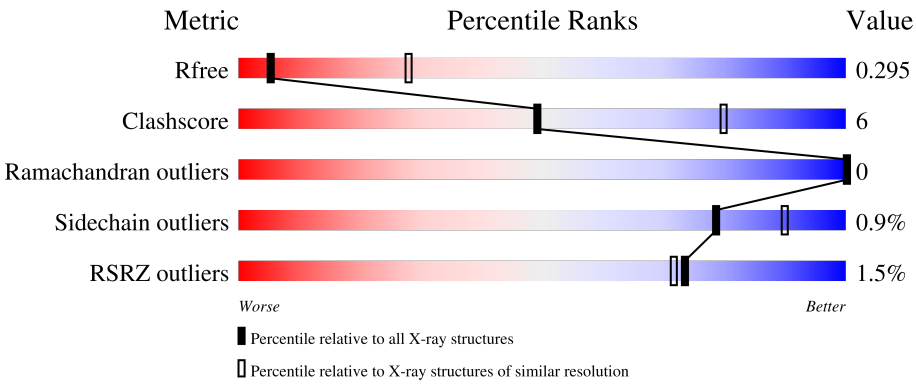
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	308	84% 14% •
2	B	171	% 71% 15% 14%
3	C	307	86% 10% 5%
4	D	219	5% 43% 6% 50%
5	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	F	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6845 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 Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2368	1492	391	473	12	0	0	0

- Molecule 2 is a protein called Interleukin-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	147	1133	719	201	207	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	GLY	-	expression tag	UNP Q9NPF7
B	191	THR	-	expression tag	UNP Q9NPF7
B	192	LYS	-	expression tag	UNP Q9NPF7
B	193	HIS	-	expression tag	UNP Q9NPF7
B	194	HIS	-	expression tag	UNP Q9NPF7
B	195	HIS	-	expression tag	UNP Q9NPF7
B	196	HIS	-	expression tag	UNP Q9NPF7
B	197	HIS	-	expression tag	UNP Q9NPF7
B	198	HIS	-	expression tag	UNP Q9NPF7

- Molecule 3 is a protein called Interleukin-23 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	293	2369	1516	389	448	16	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	310	PRO	LEU	variant	UNP Q5VWK5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	318	ILE	-	expression tag	UNP Q5VWK5
C	319	GLU	-	expression tag	UNP Q5VWK5
C	320	GLY	-	expression tag	UNP Q5VWK5
C	321	ARG	-	expression tag	UNP Q5VWK5
C	322	GLY	-	expression tag	UNP Q5VWK5
C	323	THR	-	expression tag	UNP Q5VWK5
C	324	LYS	-	expression tag	UNP Q5VWK5
C	325	HIS	-	expression tag	UNP Q5VWK5
C	326	HIS	-	expression tag	UNP Q5VWK5
C	327	HIS	-	expression tag	UNP Q5VWK5
C	328	HIS	-	expression tag	UNP Q5VWK5
C	329	HIS	-	expression tag	UNP Q5VWK5
C	330	HIS	-	expression tag	UNP Q5VWK5

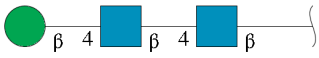
- Molecule 4 is a protein called Interleukin-12 receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	109	837	524	141	164	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	240	HIS	-	expression tag	UNP P42701
D	241	HIS	-	expression tag	UNP P42701
D	242	HIS	-	expression tag	UNP P42701
D	243	HIS	-	expression tag	UNP P42701
D	244	HIS	-	expression tag	UNP P42701
D	245	HIS	-	expression tag	UNP P42701

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



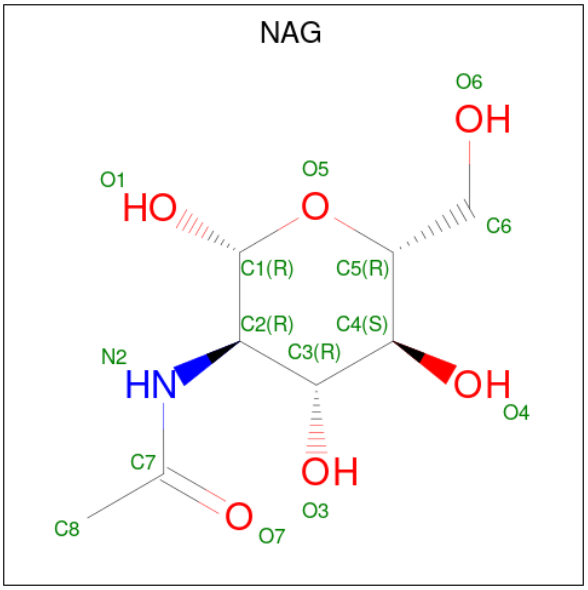
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	3	39	22	2	15	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 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		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0

- Molecule 8 is water.

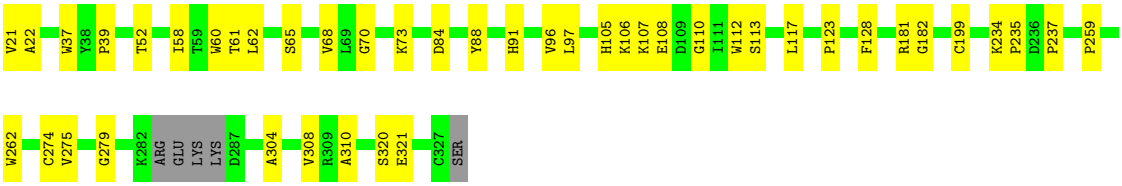
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	1	1	1	0	0

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.

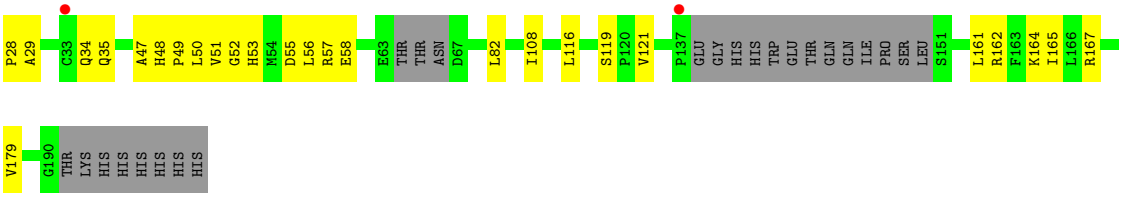
- Molecule 1: Interleukin-12 subunit beta

Chain A:



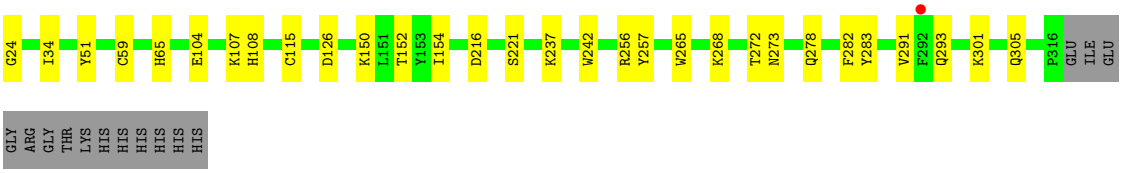
- Molecule 2: Interleukin-23 subunit alpha

Chain B:



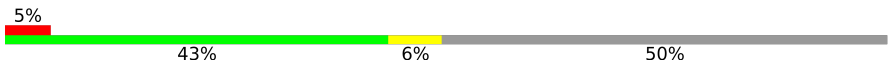
- Molecule 3: Interleukin-23 receptor

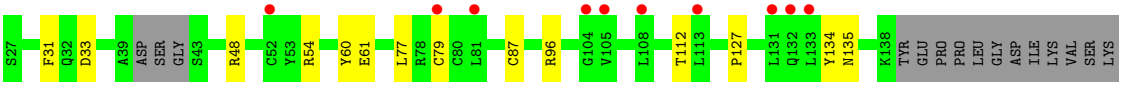
Chain C:



- Molecule 4: Interleukin-12 receptor subunit beta-1

Chain D:





LEU ALA GLY GLN LEU ARG MET GLU TRP GLU THR PRO ASP ASN GLN VAL GLY ALA GLU VAL GLN PHE ARG HIS ARG THR PRO SER SER PRO TRP LYS LEU GLY ASP CYS GLY PRO GLN ASP ASP THR GLU SER CYS LEU CYS PRO LEU GLU MET ASN VAL ALA GLN GLU PHE GLN LEU

ARG ARG ARG GLN LEU GLY SER GLN GLY SER SER TRP SER LYS TRP SER SER PRO VAL CYS VAL PRO PRO GLU ASN PRO PRO GLN PRO HIS HIS HIS HIS HIS HIS

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 33% 67%

NAG1 NAG2 BMA3

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1 NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.71Å 118.48Å 186.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 3.40 47.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.7 (47.99-3.40) 89.7 (47.99-3.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.238 , 0.295 0.238 , 0.295	Depositor DCC
R_{free} test set	1948 reflections (9.15%)	wwPDB-VP
Wilson B-factor (Å^2)	146.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 86.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6845	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: BMA, NAG

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	0.24	0/2424	0.46	0/3300
2	B	0.24	0/1160	0.41	0/1574
3	C	0.25	0/2433	0.46	0/3313
4	D	0.24	0/859	0.43	0/1170
All	All	0.24	0/6876	0.45	0/9357

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	2368	0	2240	36	0
2	B	1133	0	1111	15	0
3	C	2369	0	2263	20	0
4	D	837	0	761	9	0
5	E	39	0	34	0	0
6	F	28	0	25	0	0
7	A	14	0	13	4	0
7	C	56	0	52	2	0
8	A	1	0	0	0	0
All	All	6845	0	6499	78	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 6.

The worst 5 of 78 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:21:VAL:HG23	1:A:22:ALA:H	1.21	1.00
1:A:52:THR:HG23	1:A:73:LYS:HE2	1.67	0.77
1:A:52:THR:HB	1:A:97:LEU:HD23	1.69	0.73
7:C:405:NAG:H83	7:C:405:NAG:H3	1.71	0.73
1:A:21:VAL:HG23	1:A:22:ALA:N	2.02	0.72

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	299/308 (97%)	285 (95%)	14 (5%)	0	100	100
2	B	141/171 (82%)	134 (95%)	7 (5%)	0	100	100
3	C	291/307 (95%)	270 (93%)	21 (7%)	0	100	100
4	D	105/219 (48%)	99 (94%)	6 (6%)	0	100	100
All	All	836/1005 (83%)	788 (94%)	48 (6%)	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	264/278 (95%)	263 (100%)	1 (0%)	91	95
2	B	123/147 (84%)	120 (98%)	3 (2%)	49	74
3	C	261/278 (94%)	259 (99%)	2 (1%)	81	91
4	D	91/194 (47%)	90 (99%)	1 (1%)	73	86
All	All	739/897 (82%)	732 (99%)	7 (1%)	78	90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	ARG
3	C	59	CYS
4	D	77	LEU
3	C	115	CYS
2	B	56	LEU

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	105	HIS
3	C	65	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)

5 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	$\#\|Z\| > 2$
5	NAG	E	1	5,1	14,14,15	0.38	0	17,19,21	0.88	0
5	NAG	E	2	5	14,14,15	0.76	1 (7%)	17,19,21	0.89	0
5	BMA	E	3	5	11,11,12	1.00	2 (18%)	15,15,17	1.50	3 (20%)
6	NAG	F	1	6,3	14,14,15	0.52	0	17,19,21	0.53	0
6	NAG	F	2	6	14,14,15	0.35	0	17,19,21	0.53	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	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	O5-C1	-2.54	1.39	1.43
5	E	3	BMA	C4-C5	2.23	1.57	1.53
5	E	3	BMA	C4-C3	2.09	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3	BMA	C1-C2-C3	-3.26	105.66	109.67
5	E	3	BMA	O5-C1-C2	-2.76	106.51	110.77
5	E	3	BMA	C3-C4-C5	2.39	114.50	110.24

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C1-C2-N2-C7

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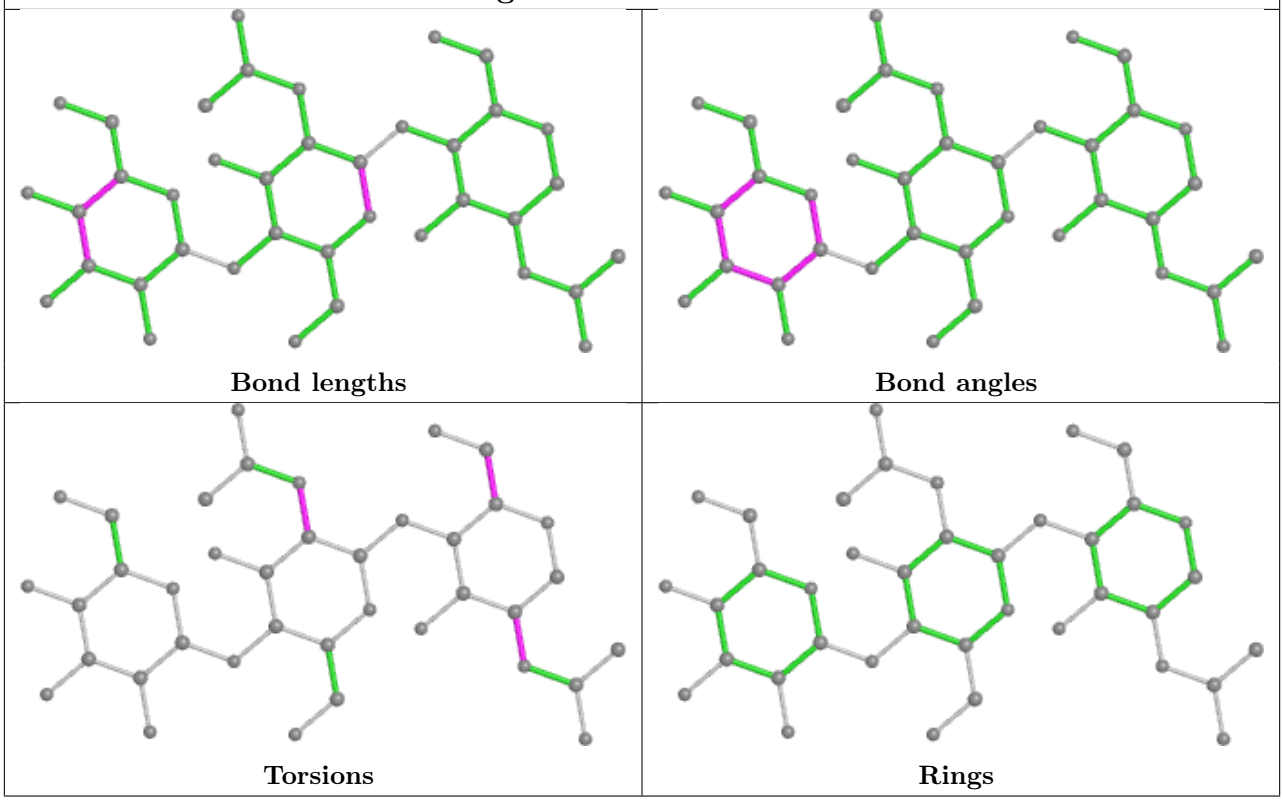
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C1-C2-N2-C7
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
6	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

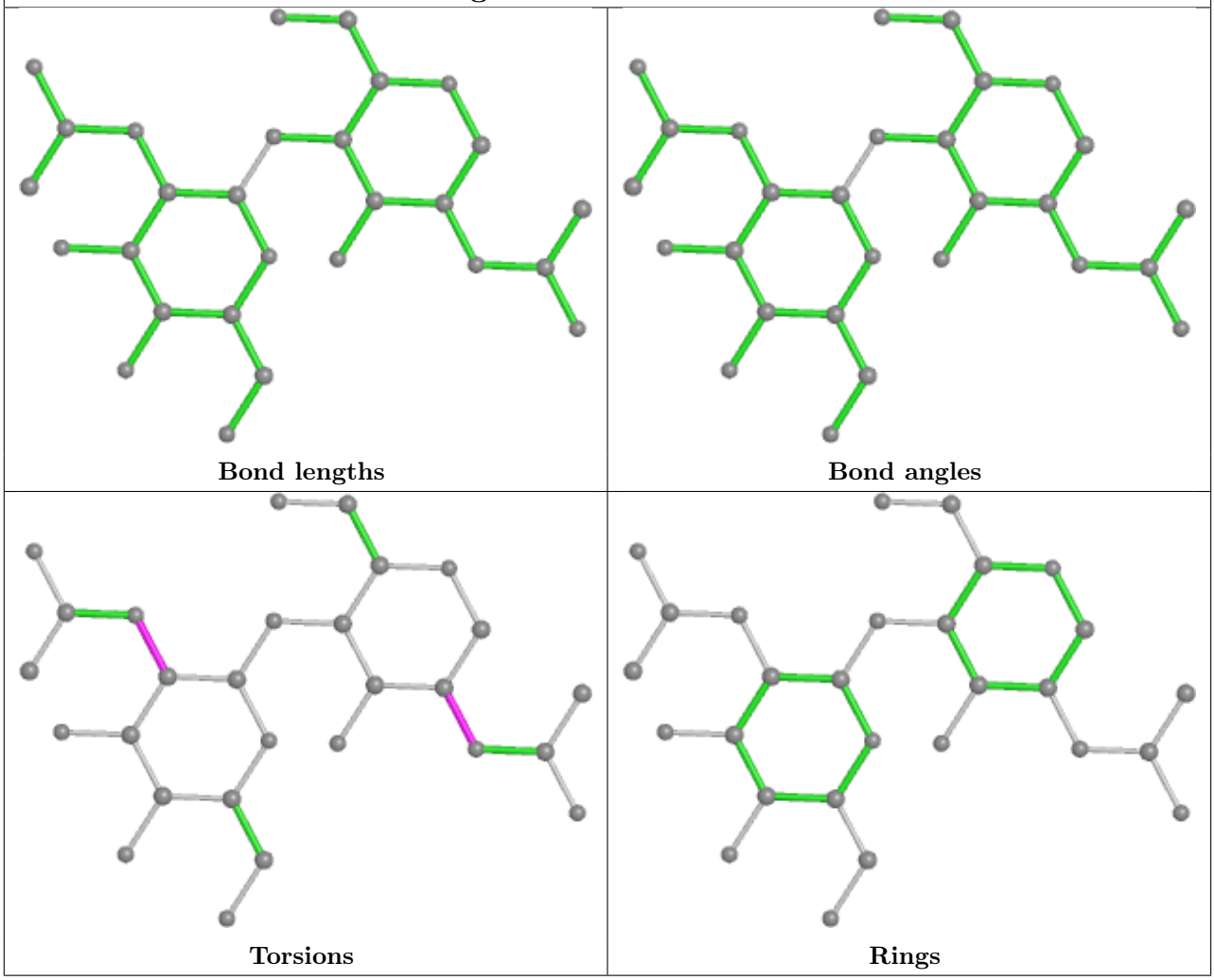
No monomer is involved in short contacts.

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 E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
7	NAG	C	402	3	14,14,15	0.24	0	17,19,21	0.50	0
7	NAG	C	406	3	14,14,15	0.19	0	17,19,21	0.42	0
7	NAG	C	401	3	14,14,15	0.30	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	C	405	3	14,14,15	1.00	1 (7%)	17,19,21	1.20	2 (11%)
7	NAG	A	401	1	14,14,15	0.70	1 (7%)	17,19,21	0.60	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
7	NAG	C	402	3	-	2/6/23/26	0/1/1/1
7	NAG	C	406	3	-	2/6/23/26	0/1/1/1
7	NAG	C	401	3	-	2/6/23/26	0/1/1/1
7	NAG	C	405	3	-	4/6/23/26	0/1/1/1
7	NAG	A	401	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	405	NAG	O5-C1	2.87	1.48	1.43
7	A	401	NAG	C1-C2	2.42	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	405	NAG	C2-N2-C7	3.23	127.51	122.90
7	C	405	NAG	C1-O5-C5	-2.47	108.84	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	C1-C2-N2-C7
7	A	401	NAG	C4-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	C	406	NAG	O5-C5-C6-O6
7	C	405	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	405	NAG	2	0
7	A	401	NAG	4	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	303/308 (98%)	0.01	0 100 100	105, 147, 247, 298	0
2	B	147/171 (85%)	-0.12	2 (1%) 75 74	101, 153, 210, 270	0
3	C	293/307 (95%)	-0.09	1 (0%) 94 93	95, 139, 194, 219	0
4	D	109/219 (49%)	0.14	10 (9%) 9 10	136, 175, 218, 230	0
All	All	852/1005 (84%)	-0.03	13 (1%) 73 72	95, 150, 223, 298	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	137	PRO	3.9
4	D	105	VAL	3.8
4	D	132	GLN	3.0
4	D	113	LEU	2.7
4	D	133	LEU	2.7

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
5	BMA	E	3	11/12	0.72	0.19	205,239,249,251	0
5	NAG	E	2	14/15	0.73	0.16	151,205,219,219	0

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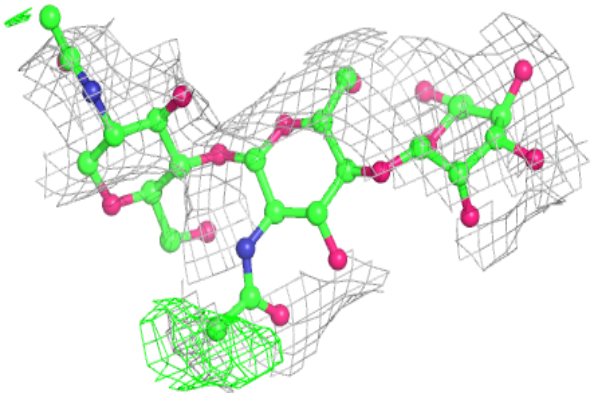
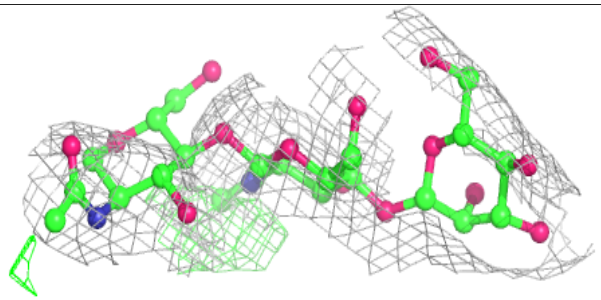
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	E	1	14/15	0.77	0.28	212,254,271,278	0
6	NAG	F	2	14/15	0.88	0.22	205,211,223,228	0
6	NAG	F	1	14/15	0.93	0.14	132,192,214,219	0

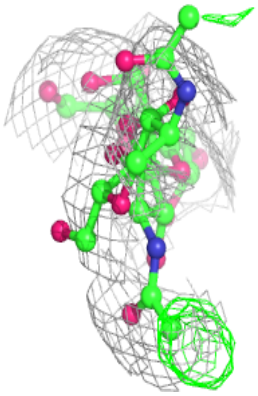
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

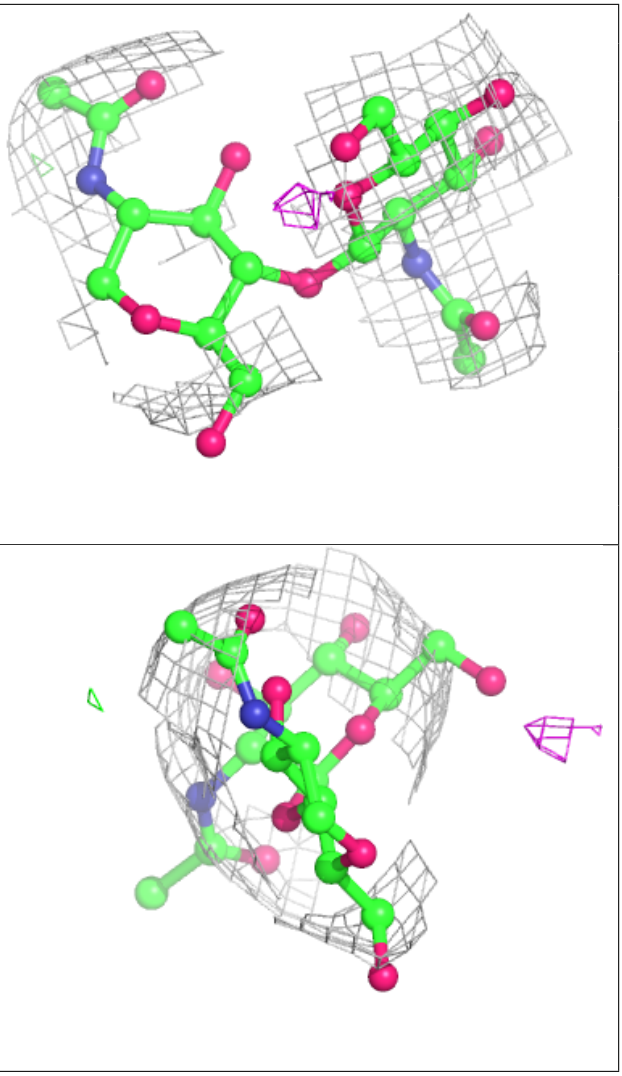






Electron density around Chain F:

$2mF_o$-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
7	NAG	C	405	14/15	0.82	0.21	162,200,222,224	0
7	NAG	A	401	14/15	0.86	0.19	223,236,272,279	0
7	NAG	C	402	14/15	0.89	0.32	198,212,244,245	0
7	NAG	C	401	14/15	0.90	0.22	134,176,208,226	0
7	NAG	C	406	14/15	0.90	0.22	134,154,192,201	0

6.5 Other polymers (i)

There are no such residues in this entry.