Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 09:49 AM EDT

PDB ID	:	5XAU
Title	:	Crystal structure of integrin binding fragment of laminin-511
Authors	:	Takizawa, M.; Arimori, T.; Kitago, Y.; Takagi, J.; Sekiguchi, K.
Deposited on	:	2017-03-15
Resolution	:	1.80 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 (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:

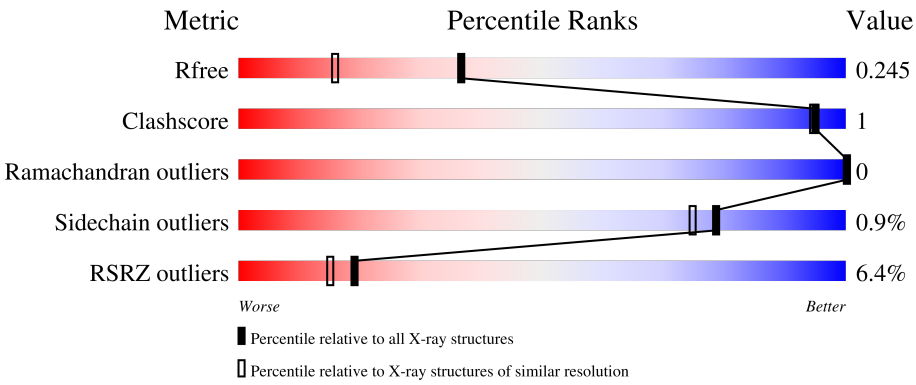
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	674	3% 86% • 11%
1	D	674	4% 84% • 12%
2	B	74	11% 95% • •
2	E	74	34% 92% 5% •
3	C	83	6% 82% •• 16%

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Mol	Chain	Length	Quality of chain
3	F	83	11% 60% • 37%
4	G	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11975 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 Laminin subunit alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	600	4550	2885	799	848	18	0	1	0
1	D	594	4560	2899	794	850	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2654	GLY	-	expression tag	UNP O15230
A	2723	CYS	ILE	engineered mutation	UNP O15230
D	2654	GLY	-	expression tag	UNP O15230
D	2723	CYS	ILE	engineered mutation	UNP O15230

- Molecule 2 is a protein called Laminin subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	71	580	359	106	113	2	0	0	0
2	E	72	585	362	107	114	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1713	GLY	-	expression tag	UNP P07942
E	1713	GLY	-	expression tag	UNP P07942

- Molecule 3 is a protein called Laminin subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	70	560	342	97	116	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	52	421	257	74	86	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1527	GLY	-	expression tag	UNP P11047
C	1585	CYS	ASP	engineered mutation	UNP P11047
F	1527	GLY	-	expression tag	UNP P11047
F	1585	CYS	ASP	engineered mutation	UNP P11047

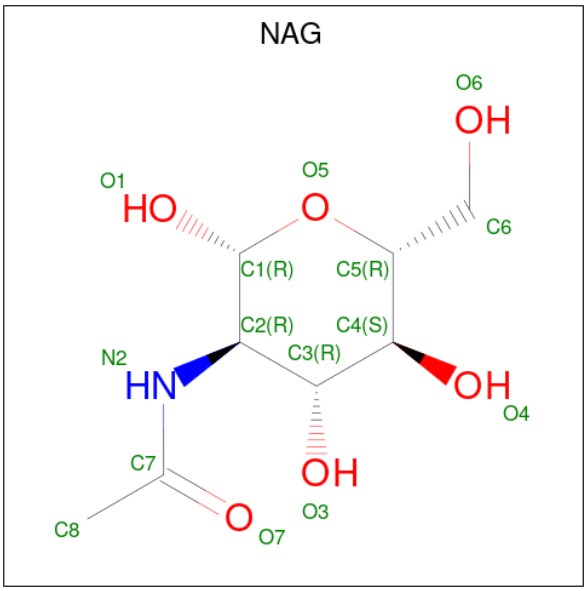
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0
			Total	Ca		
5	D	1	1	1	0	0

- Molecule 6 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		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	260	260	260	0	0
			Total	O		
7	B	24	24	24	0	0
			Total	O		
7	C	19	19	19	0	0
			Total	O		
7	D	256	256	256	0	0
			Total	O		
7	E	12	12	12	0	0

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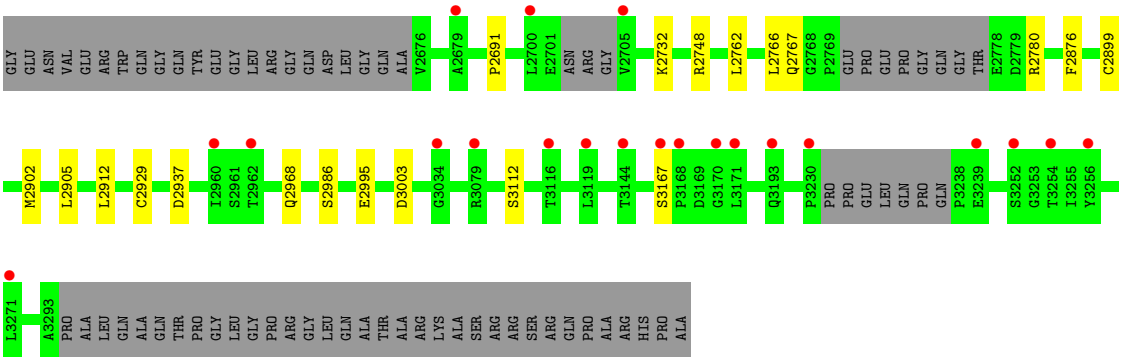
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	F	20	20	20	0	0

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.

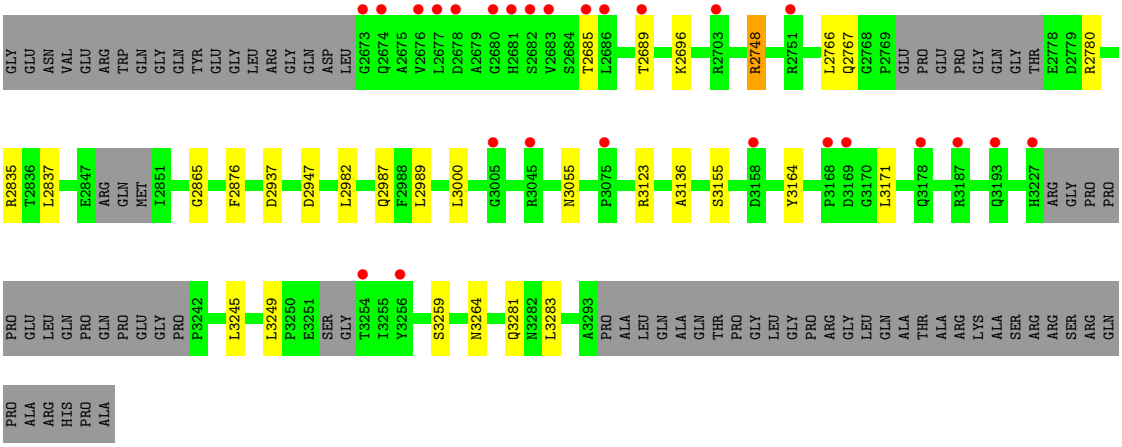
• Molecule 1: Laminin subunit alpha-5

Chain A:



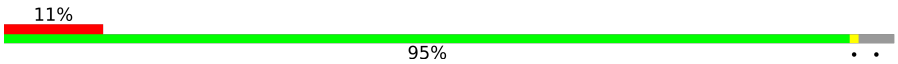
• Molecule 1: Laminin subunit alpha-5

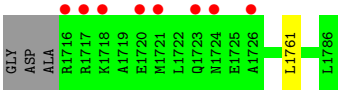
Chain D:



• Molecule 2: Laminin subunit beta-1

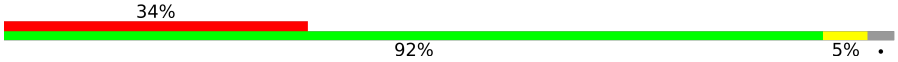
Chain B:

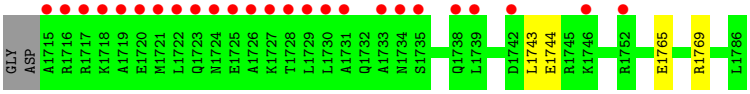




• Molecule 2: Laminin subunit beta-1

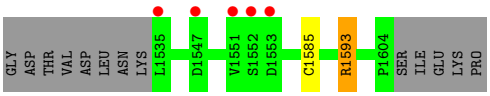
Chain E:





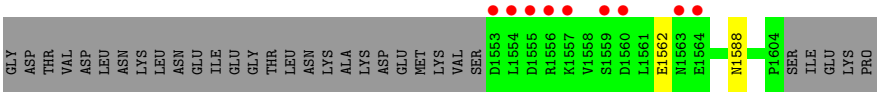
• Molecule 3: Laminin subunit gamma-1

Chain C:



• Molecule 3: Laminin subunit gamma-1

Chain F:



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

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.03Å 121.62Å 107.55Å 90.00° 127.57° 90.00°	Depositor
Resolution (Å)	49.41 – 1.80 49.41 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.41-1.80) 99.8 (49.41-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.237 0.210 , 0.245	Depositor DCC
R_{free} test set	8245 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, CA

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	0.59	0/4645	0.80	5/6300 (0.1%)
1	D	0.59	0/4653	0.81	6/6305 (0.1%)
2	B	0.52	0/582	0.69	0/776
2	E	0.58	0/587	0.72	0/783
3	C	0.58	0/563	0.74	2/752 (0.3%)
3	F	0.52	0/424	0.73	0/567
All	All	0.58	0/11454	0.79	13/15483 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2780	ARG	NE-CZ-NH2	8.08	124.34	120.30
3	C	1593	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	2780	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	D	2835	ARG	NE-CZ-NH2	-6.31	117.14	120.30
3	C	1593	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	D	2835	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	2748	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	2691	PRO	N-CA-CB	5.83	110.30	103.30
1	D	2780	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	2937	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	2947	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	2748	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	3003	ASP	CB-CG-OD1	5.21	122.99	118.30

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	4550	0	4447	7	0
1	D	4560	0	4547	16	0
2	B	580	0	604	0	0
2	E	585	0	609	3	0
3	C	560	0	560	1	0
3	F	421	0	416	3	0
4	G	28	0	25	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	42	0	39	0	0
6	D	56	0	52	0	0
7	A	260	0	0	0	0
7	B	24	0	0	0	0
7	C	19	0	0	1	0
7	D	256	0	0	1	0
7	E	12	0	0	0	0
7	F	20	0	0	0	0
All	All	11975	0	11299	26	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 1.

All (26) 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:D:2748:ARG:HH22	3:F:1588:ASN:HD21	1.13	0.93
1:D:3123:ARG:HH21	1:D:3264:ASN:HD21	1.27	0.82
1:A:2767[B]:GLN:HE21	1:A:2899:CYS:H	1.42	0.66
1:D:2685:THR:O	1:D:2689:THR:HG23	2.04	0.58
1:A:2762:LEU:HD13	1:A:2905:LEU:HD13	1.91	0.53
1:A:2732:LYS:HD2	1:A:3112:SER:HB3	1.93	0.51
1:D:3245:LEU:HD13	1:D:3249:LEU:HD23	1.93	0.50
1:D:3164:TYR:CZ	1:D:3171:LEU:HD11	2.47	0.49
2:E:1765:GLU:O	2:E:1769:ARG:HG3	2.13	0.49
1:D:2748:ARG:HH22	3:F:1588:ASN:ND2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3136:ALA:HB2	1:D:3283:LEU:HD11	1.96	0.48
1:A:2767[A]:GLN:NE2	1:A:2929:CYS:SG	2.89	0.46
1:D:3281:GLN:NE2	7:D:3508:HOH:O	2.48	0.46
1:A:2995:GLU:HG3	1:A:2995:GLU:O	2.16	0.45
1:D:2989:LEU:CD1	1:D:3000:LEU:HD11	2.49	0.43
1:A:2902:MET:HG2	1:A:2912:LEU:CD2	2.48	0.43
1:D:3155:SER:HB2	1:D:3259:SER:O	2.19	0.43
1:D:2837:LEU:HA	1:D:2865:GLY:O	2.18	0.43
1:D:3164:TYR:CE2	1:D:3171:LEU:HD11	2.53	0.43
1:A:2902:MET:HG2	1:A:2912:LEU:HG	2.00	0.42
3:C:1593:ARG:HD2	7:C:1706:HOH:O	2.19	0.42
1:D:2696:LYS:HD2	2:E:1744:GLU:OE1	2.19	0.41
1:D:2987:GLN:HE22	1:D:3055:ASN:HA	1.86	0.41
1:D:2982:LEU:C	1:D:2982:LEU:HD23	2.42	0.41
2:E:1743:LEU:HD21	3:F:1562:GLU:HG3	2.04	0.40
1:D:2989:LEU:HD11	1:D:3000:LEU:HD11	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	593/674 (88%)	581 (98%)	12 (2%)	0	100	100
1	D	584/674 (87%)	573 (98%)	11 (2%)	0	100	100
2	B	69/74 (93%)	69 (100%)	0	0	100	100
2	E	70/74 (95%)	70 (100%)	0	0	100	100
3	C	68/83 (82%)	68 (100%)	0	0	100	100
3	F	50/83 (60%)	50 (100%)	0	0	100	100
All	All	1434/1662 (86%)	1411 (98%)	23 (2%)	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	473/550 (86%)	467 (99%)	6 (1%)	69	62
1	D	489/550 (89%)	486 (99%)	3 (1%)	86	84
2	B	63/64 (98%)	62 (98%)	1 (2%)	62	54
2	E	63/64 (98%)	63 (100%)	0	100	100
3	C	64/76 (84%)	63 (98%)	1 (2%)	62	54
3	F	48/76 (63%)	48 (100%)	0	100	100
All	All	1200/1380 (87%)	1189 (99%)	11 (1%)	78	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2766	LEU
1	A	2876	PHE
1	A	2937	ASP
1	A	2968	GLN
1	A	2986	SER
1	A	3167	SER
2	B	1761	LEU
3	C	1585	CYS
1	D	2766	LEU
1	D	2767	GLN
1	D	2876	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2827	GLN
1	A	2984	GLN
1	A	3053	GLN

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Mol	Chain	Res	Type
1	A	3139	ASN
1	A	3177	GLN
1	A	3268	GLN
1	D	2987	GLN
1	D	3128	HIS
1	D	3264	ASN
1	D	3281	GLN
2	E	1750	ASN
3	F	1563	ASN
3	F	1568	GLN
3	F	1588	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	G	1	1,4	14,14,15	0.28	0	17,19,21	1.17	3 (17%)
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	0.75	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	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	O5-C5-C6	2.39	110.95	107.20
4	G	1	NAG	C1-O5-C5	2.21	115.18	112.19
4	G	1	NAG	O5-C1-C2	-2.09	107.98	111.29

There are no chirality outliers.

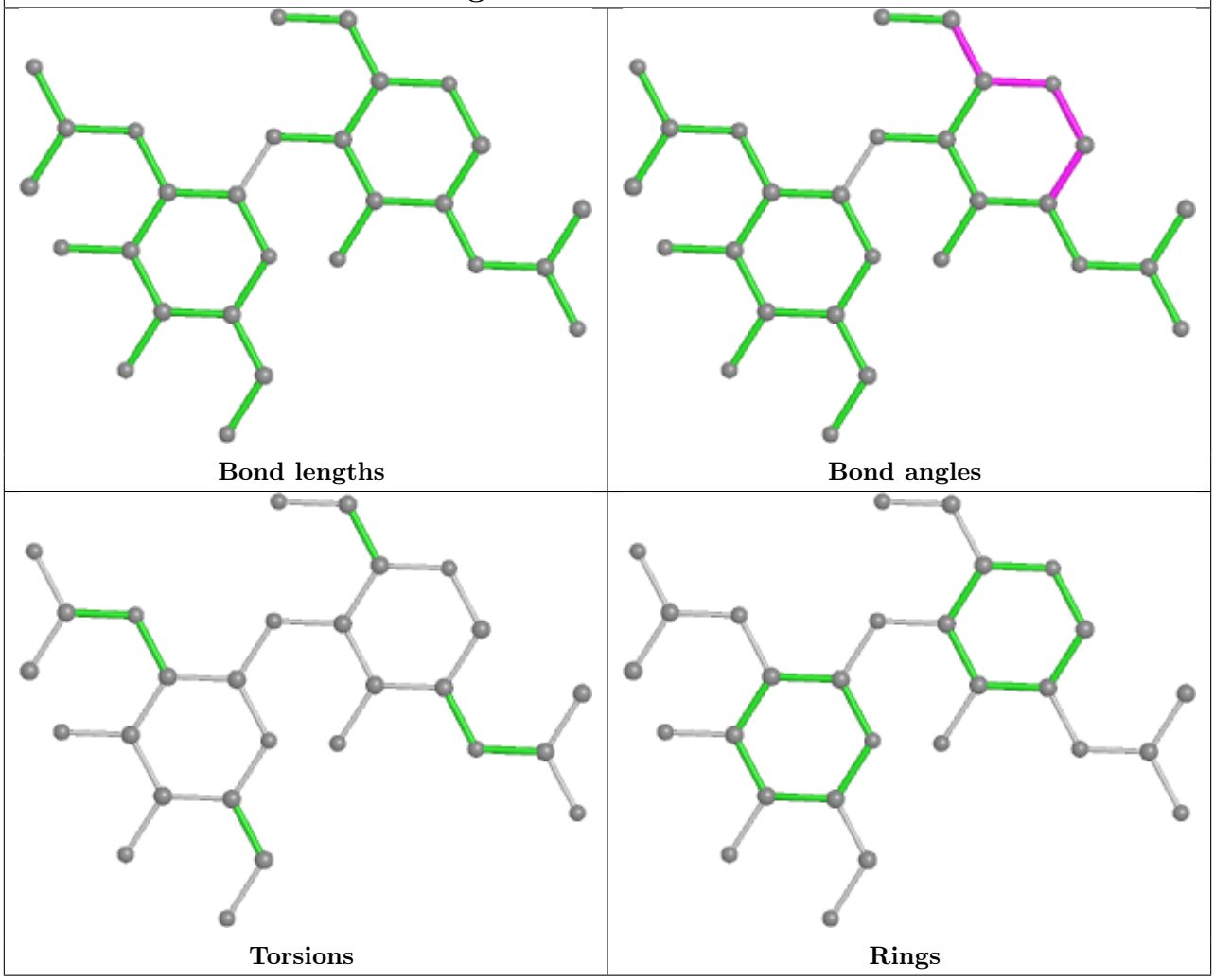
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	NAG	A	3403	1	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
6	NAG	D	3403	1	14,14,15	0.45	0	17,19,21	1.33	1 (5%)
6	NAG	D	3402	1	14,14,15	0.41	0	17,19,21	1.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	D	3405	1	14,14,15	0.38	0	17,19,21	1.06	2 (11%)
6	NAG	D	3404	1	14,14,15	0.33	0	17,19,21	0.69	0
6	NAG	A	3404	1	14,14,15	0.33	0	17,19,21	0.60	0
6	NAG	A	3402	1	14,14,15	0.45	0	17,19,21	1.21	3 (17%)

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
6	NAG	A	3403	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3403	1	-	2/6/23/26	0/1/1/1
6	NAG	D	3402	1	-	2/6/23/26	0/1/1/1
6	NAG	D	3405	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3402	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	3402	NAG	C1-O5-C5	6.18	120.57	112.19
6	D	3403	NAG	O5-C1-C2	-3.94	105.06	111.29
6	D	3405	NAG	C1-O5-C5	3.16	116.47	112.19
6	A	3402	NAG	C2-N2-C7	2.55	126.53	122.90
6	A	3403	NAG	O5-C1-C2	-2.29	107.67	111.29
6	A	3402	NAG	C8-C7-N2	2.15	119.74	116.10
6	A	3402	NAG	O5-C5-C6	2.13	110.54	107.20
6	D	3405	NAG	O5-C5-C6	2.07	110.45	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3402	NAG	O5-C5-C6-O6
6	A	3402	NAG	C4-C5-C6-O6
6	A	3402	NAG	C8-C7-N2-C2
6	A	3402	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	D	3402	NAG	C4-C5-C6-O6
6	D	3403	NAG	C4-C5-C6-O6
6	D	3403	NAG	O5-C5-C6-O6
6	D	3402	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	600/674 (89%)	0.08	21 (3%) 44 38	18, 31, 57, 72	0
1	D	594/674 (88%)	0.14	26 (4%) 34 28	19, 31, 53, 73	0
2	B	71/74 (95%)	0.30	8 (11%) 5 3	22, 37, 77, 93	0
2	E	72/74 (97%)	1.45	25 (34%) 0 0	21, 48, 78, 104	0
3	C	70/83 (84%)	0.41	5 (7%) 16 12	22, 37, 75, 80	0
3	F	52/83 (62%)	0.65	9 (17%) 1 1	22, 39, 86, 96	0
All	All	1459/1662 (87%)	0.22	94 (6%) 19 15	18, 32, 64, 104	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1715	ALA	7.2
1	A	2962	THR	5.9
2	E	1729	LEU	5.5
1	D	2676	VAL	5.5
2	E	1731	ALA	5.5
2	E	1725	GLU	5.3
1	D	2751	ARG	5.1
3	C	1551	VAL	4.7
2	E	1717	ARG	4.6
1	D	2681	HIS	4.5
3	F	1556	ARG	4.5
2	E	1718	LYS	4.5
3	F	1553	ASP	4.1
2	E	1730	LEU	4.1
1	D	2677	LEU	4.0
1	D	3227	HIS	4.0
1	D	2703	ARG	4.0
2	B	1716	ARG	4.0
1	A	3256	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	1726	ALA	3.8
2	E	1716	ARG	3.8
2	E	1721	MET	3.7
2	E	1738	GLN	3.6
2	E	1728	THR	3.6
1	D	2673	GLY	3.6
1	D	3187	ARG	3.6
2	B	1717	ARG	3.5
2	E	1735	SER	3.3
2	E	1723	GLN	3.3
1	A	3171	LEU	3.3
1	D	3256	TYR	3.3
3	F	1554	LEU	3.3
1	A	2679	ALA	3.3
1	A	3193	GLN	3.2
2	B	1718	LYS	3.2
2	E	1720	GLU	3.1
1	D	2689	THR	3.1
2	B	1721	MET	3.1
1	A	3119	LEU	3.0
3	C	1547	ASP	3.0
3	F	1555	ASP	3.0
3	F	1564	GLU	3.0
1	A	3230	PRO	3.0
1	D	2674	GLN	3.0
2	E	1724	ASN	3.0
2	E	1742	ASP	2.9
1	A	3079	ARG	2.9
2	E	1722	LEU	2.9
1	A	3167	SER	2.8
3	C	1552	SER	2.8
1	D	3169	ASP	2.8
2	E	1739	LEU	2.8
1	D	3254	THR	2.7
1	D	3193	GLN	2.7
1	D	2685	THR	2.7
1	A	2705	VAL	2.7
1	A	3254	THR	2.7
2	E	1733	ALA	2.6
1	A	3168	PRO	2.6
3	F	1563	ASN	2.6
1	A	3239	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	3116	THR	2.6
1	D	2683	VAL	2.6
2	B	1724	ASN	2.6
2	E	1719	ALA	2.5
1	A	3252	SER	2.5
1	A	3170	GLY	2.5
1	D	2680	GLY	2.5
1	D	3005	GLY	2.5
1	D	3168	PRO	2.4
2	E	1727	LYS	2.4
1	D	3158	ASP	2.4
3	F	1560	ASP	2.4
1	A	2960	ILE	2.4
3	C	1535	LEU	2.4
3	F	1559	SER	2.4
1	D	3178	GLN	2.2
1	D	3075	PRO	2.2
3	F	1557	LYS	2.2
2	E	1752	ARG	2.2
2	B	1723	GLN	2.2
1	A	3034	GLY	2.2
1	D	2678	ASP	2.2
1	A	2700	LEU	2.1
3	C	1553	ASP	2.1
1	D	2682	SER	2.1
2	E	1734	ASN	2.1
1	A	3271	LEU	2.1
1	D	2686	LEU	2.1
2	B	1726	ALA	2.1
1	A	3144	THR	2.1
2	B	1720	GLU	2.1
2	E	1746	LYS	2.1
1	D	3045	ARG	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)

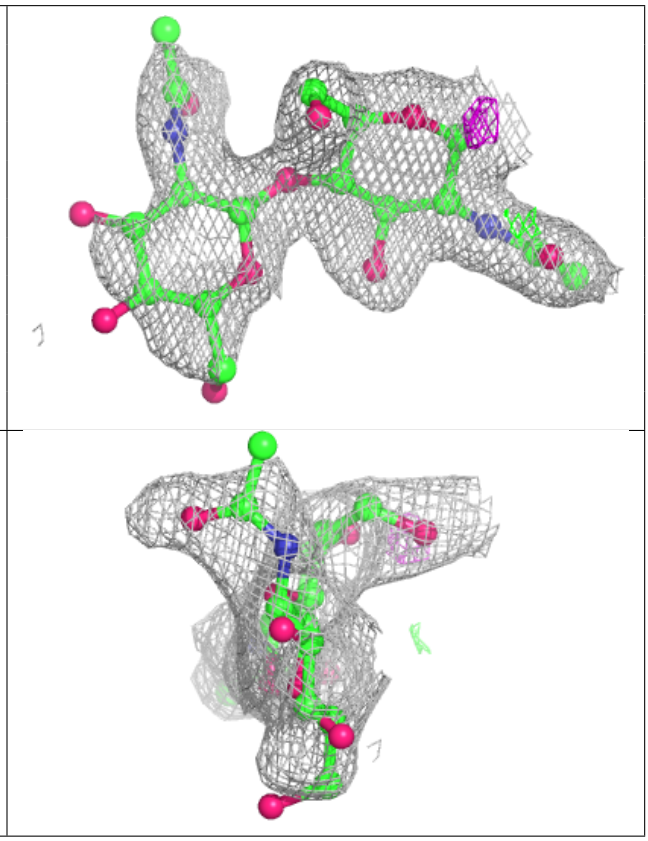
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	2	14/15	0.81	0.39	68,74,80,85	0
4	NAG	G	1	14/15	0.91	0.14	37,41,48,59	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 G:

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	NAG	A	3402	14/15	0.68	0.32	53,56,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	D	3403	14/15	0.79	0.20	57,64,69,71	0
6	NAG	D	3404	14/15	0.83	0.12	42,46,52,53	0
6	NAG	D	3405	14/15	0.83	0.12	39,45,50,53	0
6	NAG	D	3402	14/15	0.84	0.21	47,53,59,60	0
6	NAG	A	3403	14/15	0.90	0.15	44,50,56,57	0
6	NAG	A	3404	14/15	0.92	0.18	39,42,49,50	0
5	CA	A	3401	1/1	0.96	0.07	39,39,39,39	0
5	CA	D	3401	1/1	0.99	0.08	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.