



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:07 AM UTC

PDB ID : 5XAU / pdb_00005xau
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 ⓘ 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:

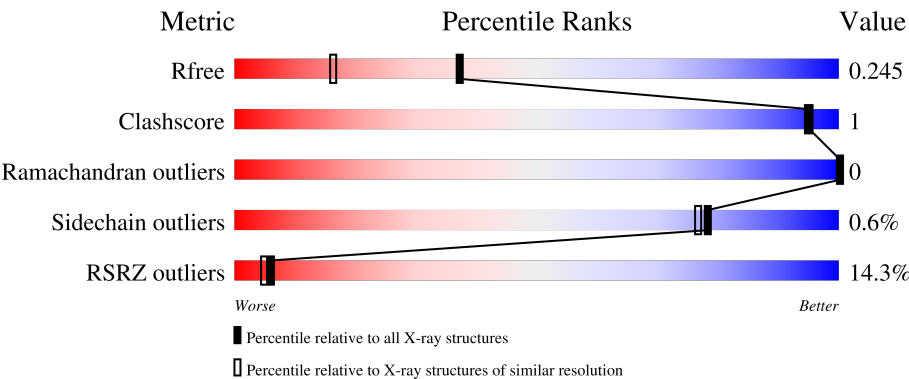
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	674	11% 86% 11%
1	D	674	8% 85% 12%
2	B	74	20% 95%
2	E	74	38% 92% 5%
3	C	83	20% 83% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	83	17% 60% 37%
4	G	2	50% 50%

2 Entry composition

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
1	A	600	Total	C	N	O	S	0	1	0
			4550	2885	799	848	18			
1	D	594	Total	C	N	O	S	0	0	0
			4560	2899	794	850	17			

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
2	B	71	Total	C	N	O	S	0	0	0
			580	359	106	113	2			
2	E	72	Total	C	N	O	S	0	0	0
			585	362	107	114	2			

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
3	C	70	Total	C	N	O	S	0	0	0
			560	342	97	116	5			

Continued on next page...

Continued from previous page...

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

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
4	G	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is water.

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

Continued on next page...

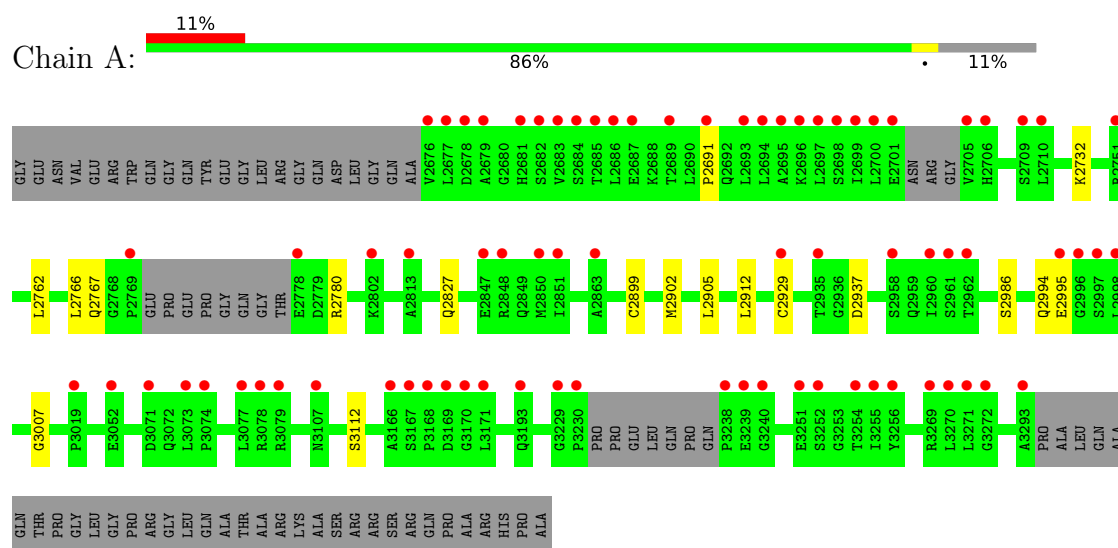
Continued from previous page...

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

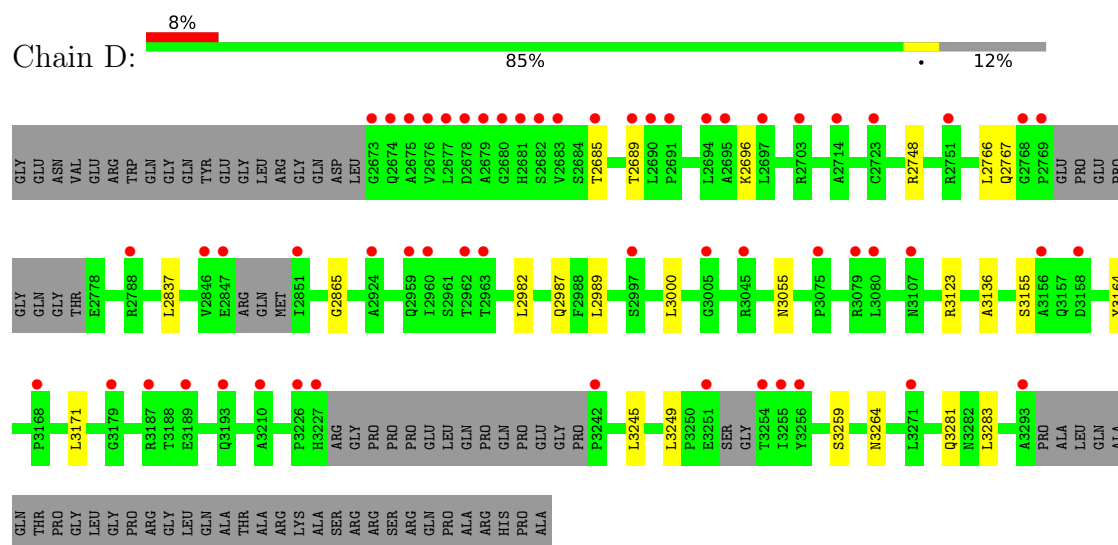
3 Residue-property plots [i](#)

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

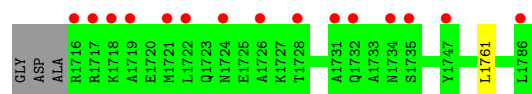


• Molecule 1: Laminin subunit alpha-5

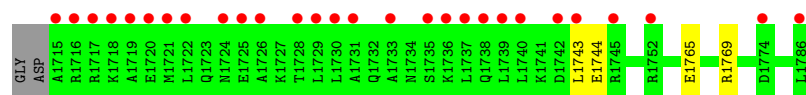
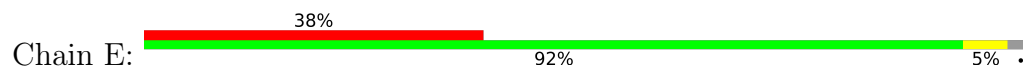


• Molecule 2: Laminin subunit beta-1

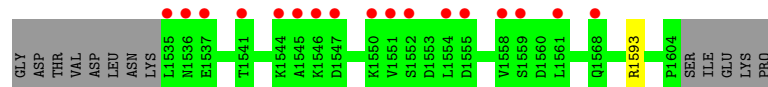
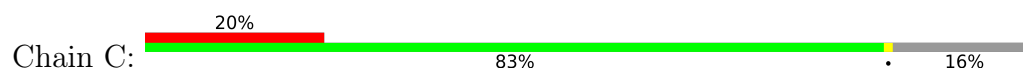




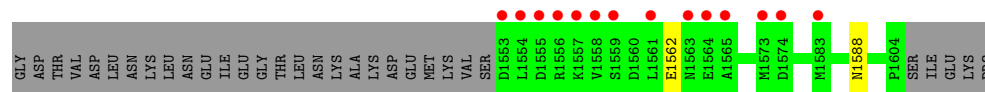
- Molecule 2: Laminin subunit beta-1



- Molecule 3: Laminin subunit gamma-1



- Molecule 3: Laminin subunit gamma-1



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.01%)	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)	0.38 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.77	1/4645 (0.0%)	0.83	2/6300 (0.0%)
1	D	0.78	0/4653	0.86	0/6305
2	B	0.70	0/582	0.94	0/776
2	E	0.74	0/587	0.96	0/783
3	C	0.76	0/563	0.89	0/752
3	F	0.70	0/424	0.95	0/567
All	All	0.77	1/11454 (0.0%)	0.86	2/15483 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3007	GLY	N-CA	5.07	1.49	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2691	PRO	N-CA-CB	6.33	110.30	103.33
1	A	2780	ARG	NE-CZ-NH2	5.71	124.34	119.20

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	8	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	27	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 (27) 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
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:D:2982:LEU:C	1:D:2982:LEU:HD23	2.42	0.45
1:A:2995:GLU:HG3	1:A:2995:GLU:O	2.16	0.45
1:A:2994:GLN:O	1:A:2995:GLU:C	2.60	0.45
1:D:2989:LEU:CD1	1:D:3000:LEU:HD11	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 ⓘ

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%)	469 (99%)	4 (1%)	73	70
1	D	489/550 (89%)	487 (100%)	2 (0%)	84	83
2	B	63/64 (98%)	62 (98%)	1 (2%)	55	47
2	E	63/64 (98%)	63 (100%)	0	100	100
3	C	64/76 (84%)	64 (100%)	0	100	100
3	F	48/76 (63%)	48 (100%)	0	100	100
All	All	1200/1380 (87%)	1193 (99%)	7 (1%)	78	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2766	LEU
1	A	2827	GLN
1	A	2937	ASP
1	A	2986	SER
2	B	1761	LEU
1	D	2766	LEU
1	D	2767	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2809	GLN
1	A	2827	GLN
1	A	2920	GLN
1	A	2984	GLN
1	A	2985	GLN
1	A	3053	GLN
1	A	3139	ASN
1	A	3173	GLN
1	A	3177	GLN
1	A	3268	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2692	GLN
1	D	2987	GLN
1	D	3128	HIS
1	D	3130	HIS
1	D	3173	GLN
1	D	3178	GLN
1	D	3264	ASN
1	D	3281	GLN
2	E	1750	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	1.11	2 (11%)
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.72	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	1	NAG	C1-O5-C5	2.24	115.18	112.19
4	G	1	NAG	O5-C1-C2	-2.14	107.98	111.29

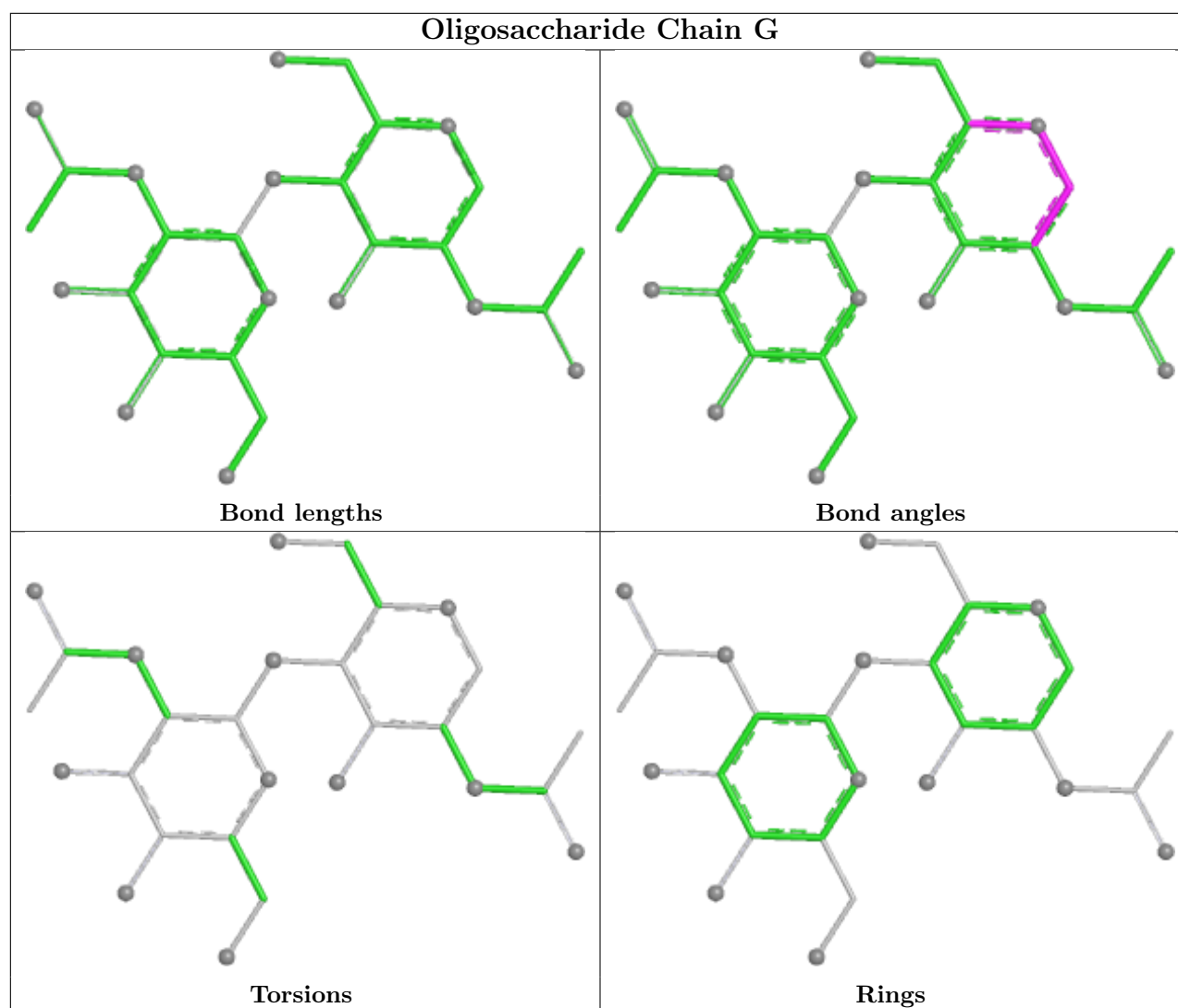
There are no chirality outliers.

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.



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	D	3403	1	14,14,15	0.47	0	17,19,21	1.32	1 (5%)
6	NAG	A	3404	1	14,14,15	0.33	0	17,19,21	0.58	0
6	NAG	D	3405	1	14,14,15	0.38	0	17,19,21	1.01	1 (5%)

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	0.41	0	17,19,21	0.77	1 (5%)
6	NAG	D	3404	1	14,14,15	0.33	0	17,19,21	0.68	0
6	NAG	A	3402	1	14,14,15	0.46	0	17,19,21	1.18	2 (11%)
6	NAG	D	3402	1	14,14,15	0.44	0	17,19,21	1.82	2 (11%)

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3402	NAG	C1-O5-C5	6.25	120.57	112.19
6	D	3403	NAG	O5-C1-C2	-4.03	105.06	111.29
6	D	3405	NAG	C1-O5-C5	3.19	116.47	112.19
6	A	3402	NAG	C2-N2-C7	2.71	126.53	122.90
6	A	3403	NAG	O5-C1-C2	-2.34	107.67	111.29
6	A	3402	NAG	C8-C7-N2	2.18	119.74	116.12
6	D	3402	NAG	C1-C2-N2	2.13	113.79	110.43

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
6	D	3402	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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

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	600/674 (89%)	0.64	77 (12%) 7 6	13, 31, 57, 72	1 (0%)
1	D	594/674 (88%)	0.55	57 (9%) 13 12	19, 31, 53, 73	0
2	B	71/74 (95%)	0.97	15 (21%) 2 2	22, 37, 77, 93	0
2	E	72/74 (97%)	1.91	28 (38%) 1 0	21, 48, 78, 104	0
3	C	70/83 (84%)	1.22	17 (24%) 2 1	22, 37, 75, 80	0
3	F	52/83 (62%)	1.23	14 (26%) 1 1	22, 39, 86, 96	0
All	All	1459/1662 (87%)	0.73	208 (14%) 6 5	13, 32, 64, 104	1 (0%)

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1715	ALA	8.2
1	A	3254	THR	5.9
1	A	2699	ILE	5.6
2	E	1731	ALA	5.6
2	E	1716	ARG	5.2
1	A	2962	THR	5.1
2	E	1729	LEU	5.1
2	E	1726	ALA	5.0
1	A	3256	TYR	5.0
1	D	3256	TYR	4.8
1	A	2700	LEU	4.8
1	A	2689	THR	4.7
2	E	1725	GLU	4.5
2	E	1737	LEU	4.5
1	A	2705	VAL	4.4
1	D	3271	LEU	4.4
2	B	1722	LEU	4.4
1	D	2689	THR	4.4
1	D	3254	THR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	2751	ARG	4.3
1	A	3238	PRO	4.3
1	D	2851	ILE	4.2
1	A	3166	ALA	4.1
3	C	1535	LEU	4.0
2	E	1728	THR	4.0
1	A	2676	VAL	4.0
1	A	2697	LEU	3.9
1	A	3293	ALA	3.9
2	E	1718	LYS	3.9
1	A	2681	HIS	3.9
2	B	1716	ARG	3.9
3	C	1554	LEU	3.9
1	A	2685	THR	3.9
1	A	3271	LEU	3.9
2	B	1721	MET	3.8
1	A	2677	LEU	3.8
1	A	2850	MET	3.8
1	D	2723	CYS	3.8
1	D	2680	GLY	3.7
2	E	1739	LEU	3.7
1	A	3252	SER	3.7
1	A	2960	ILE	3.7
2	E	1733	ALA	3.7
1	D	3227	HIS	3.6
1	A	2958	SER	3.6
3	C	1550	LYS	3.6
1	A	2691	PRO	3.6
1	A	2698	SER	3.6
3	C	1559	SER	3.6
1	D	2959	GLN	3.5
1	D	2676	VAL	3.5
2	E	1730	LEU	3.5
2	E	1738	GLN	3.4
1	A	3071	ASP	3.4
1	A	2701	GLU	3.4
3	C	1552	SER	3.4
1	D	2685	THR	3.4
1	A	3230	PRO	3.4
1	A	2706	HIS	3.3
2	E	1719	ALA	3.3
3	C	1551	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2696	LYS	3.3
3	F	1554	LEU	3.3
1	D	2681	HIS	3.2
1	D	2960	ILE	3.2
3	C	1558	VAL	3.2
1	A	3168	PRO	3.2
1	A	2682	SER	3.2
3	F	1555	ASP	3.2
1	A	2683	VAL	3.2
1	A	3193	GLN	3.2
1	A	3255	ILE	3.1
1	D	2673	GLY	3.1
2	B	1718	LYS	3.1
3	F	1557	LYS	3.1
1	D	2847	GLU	3.1
2	E	1735	SER	3.1
1	A	3170	GLY	3.1
3	F	1553	ASP	3.1
1	A	3239	GLU	3.1
3	C	1546	LYS	3.0
3	C	1547	ASP	3.0
1	A	2847	GLU	3.0
2	E	1786	LEU	3.0
1	D	3107	ASN	3.0
3	F	1561	LEU	2.9
1	A	2678	ASP	2.9
2	E	1740	LEU	2.9
1	A	2679	ALA	2.9
3	F	1559	SER	2.8
1	A	2693	LEU	2.8
2	E	1752	ARG	2.8
1	D	2675	ALA	2.8
1	D	3293	ALA	2.8
2	B	1726	ALA	2.8
1	D	3005	GLY	2.8
1	A	3251	GLU	2.8
1	D	3168	PRO	2.8
2	B	1724	ASN	2.7
1	D	2697	LEU	2.7
2	E	1722	LEU	2.7
1	A	2997	SER	2.7
1	A	3079	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	1563	ASN	2.7
1	D	2695	ALA	2.7
1	A	3019	PRO	2.7
1	D	2769	PRO	2.7
3	C	1536	ASN	2.7
1	D	3158	ASP	2.7
1	A	3167	SER	2.7
3	F	1558	VAL	2.7
1	D	3210	ALA	2.6
3	C	1541	THR	2.6
1	A	3171	LEU	2.6
2	E	1724	ASN	2.6
2	B	1786	LEU	2.6
1	A	2996	GLY	2.6
1	A	2684	SER	2.6
1	A	2709	SER	2.6
1	D	3251	GLU	2.5
1	A	2851	ILE	2.5
1	D	2768	GLY	2.5
2	E	1736	LYS	2.5
3	C	1544	LYS	2.5
1	D	3079	ARG	2.5
3	F	1556	ARG	2.5
3	F	1583	MET	2.5
2	B	1747	TYR	2.5
2	E	1743	LEU	2.5
1	D	2703	ARG	2.5
1	D	2683	VAL	2.5
3	C	1568	GLN	2.5
3	F	1574	ASP	2.5
1	A	3240	GLY	2.5
1	A	3272	GLY	2.5
1	D	2788	ARG	2.5
1	D	2678	ASP	2.5
2	E	1742	ASP	2.5
1	A	2751	ARG	2.4
1	A	3107	ASN	2.4
1	D	3242	PRO	2.4
2	E	1717	ARG	2.4
1	A	2929	CYS	2.4
3	C	1537	GLU	2.4
1	A	3270	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	2677	LEU	2.4
1	D	2997	SER	2.4
1	A	3073	LEU	2.4
1	D	2962	THR	2.4
1	A	2778	GLU	2.3
1	A	2935	THR	2.3
3	F	1564	GLU	2.3
1	A	3169	ASP	2.3
1	A	2998	LEU	2.3
1	D	2690	LEU	2.3
1	D	2691	PRO	2.3
1	D	3179	GLY	2.3
1	A	2710	LEU	2.3
3	C	1545	ALA	2.3
1	D	3255	ILE	2.3
3	C	1555	ASP	2.3
1	D	2674	GLN	2.3
3	F	1573	MET	2.3
1	D	2679	ALA	2.2
1	D	3080	LEU	2.2
1	A	2961	SER	2.2
1	D	2682	SER	2.2
1	A	2813	ALA	2.2
2	E	1745	ARG	2.2
1	D	2846	VAL	2.2
1	A	2995	GLU	2.2
1	D	3226	PRO	2.2
3	F	1565	ALA	2.2
2	E	1720	GLU	2.2
1	D	3193	GLN	2.2
2	E	1721	MET	2.1
2	B	1735	SER	2.1
1	D	3075	PRO	2.1
1	D	3189	GLU	2.1
1	A	2863	ALA	2.1
1	D	2924	ALA	2.1
2	B	1734	ASN	2.1
1	D	2963	THR	2.1
1	A	2802	LYS	2.1
1	A	3077	LEU	2.1
1	D	3045	ARG	2.1
2	B	1717	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2686	LEU	2.1
1	A	2694	LEU	2.1
1	A	2695	ALA	2.1
1	D	3156	ALA	2.1
2	E	1774	ASP	2.1
1	A	2848	ARG	2.1
1	A	3078	ARG	2.1
1	D	3187	ARG	2.1
1	A	2687	GLU	2.0
1	A	3052	GLU	2.0
2	B	1728	THR	2.0
1	A	3229	GLY	2.0
2	B	1732	GLN	2.0
1	A	2769	PRO	2.0
1	A	3074	PRO	2.0
1	D	2694	LEU	2.0
3	C	1561	LEU	2.0
1	D	2714	ALA	2.0
2	B	1719	ALA	2.0
2	B	1731	ALA	2.0
1	A	3269	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

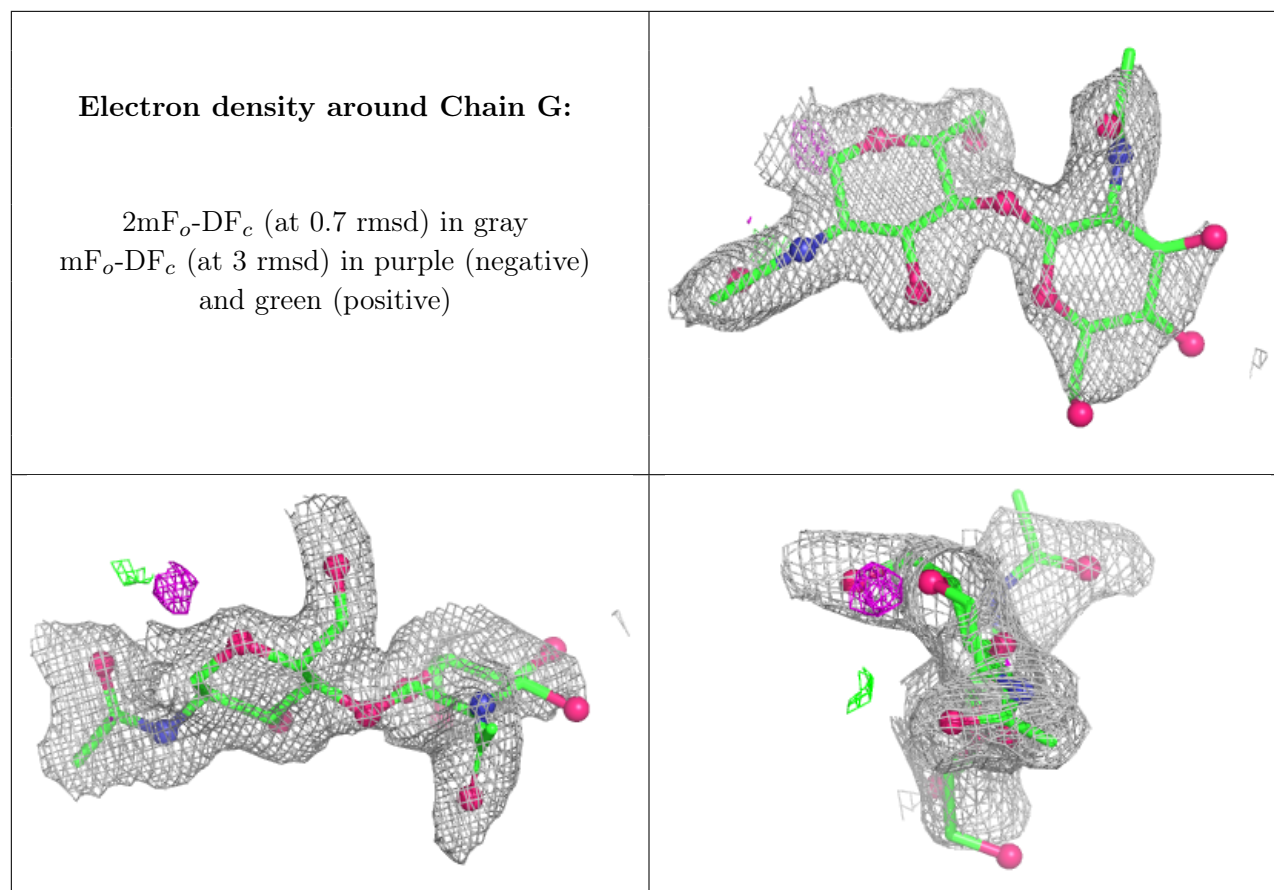
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	G	2	14/15	0.65	0.14	68,74,80,85	0
4	NAG	G	1	14/15	0.89	0.11	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.



6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
6	NAG	A	3402	14/15	0.62	0.17	53,56,58,62	0
6	NAG	D	3403	14/15	0.72	0.15	57,64,69,71	0
6	NAG	D	3402	14/15	0.78	0.13	47,53,59,60	0
6	NAG	D	3404	14/15	0.82	0.12	42,46,52,53	0
6	NAG	D	3405	14/15	0.82	0.15	39,45,50,53	0
6	NAG	A	3403	14/15	0.83	0.12	44,50,56,57	0
6	NAG	A	3404	14/15	0.87	0.10	39,42,49,50	0
5	CA	A	3401	1/1	0.95	0.07	39,39,39,39	0
5	CA	D	3401	1/1	0.98	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.