wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2026 – 06:14 PM EDT

PDB ID	:	9YOA / pdb_00009yoa
Title	:	Crystal structure of integrin a4b1 headpiece in complex with Bio-1211 (Mn)
Authors	:	Monroy, M.F.; Lin, F.Y.; Qiao, Q.
Deposited on	:	2025-10-13
Resolution	:	2.64 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:

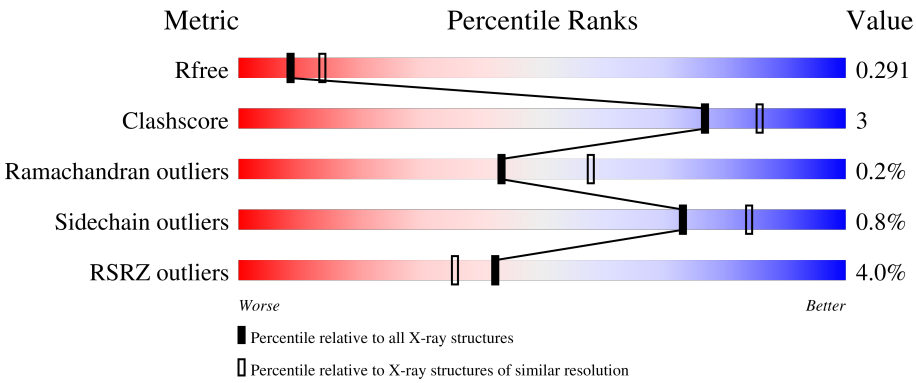
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	597	2% 93% 5% •
2	B	490	7% 90% • 7%
3	D	5	20% 20% 20% 60%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16491 atoms, of which 8124 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 Integrin alpha-4,Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	588	8970	2858	4439	785	866	22	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	TYR	conflict	UNP P13612
A	589	GLY	-	expression tag	UNP P06756
A	590	GLY	-	expression tag	UNP P06756
A	591	SER	-	expression tag	UNP P06756
A	592	GLU	-	expression tag	UNP P06756
A	593	ASN	-	expression tag	UNP P06756
A	594	LEU	-	expression tag	UNP P06756
A	595	TYR	-	expression tag	UNP P06756
A	596	PHE	-	expression tag	UNP P06756
A	597	GLN	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	455	6874	2181	3369	591	703	30	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	conflict	UNP P05556
B	195	THR	SER	conflict	UNP P05556
B	482	GLY	-	expression tag	UNP P05556
B	483	GLY	-	expression tag	UNP P05556
B	484	SER	-	expression tag	UNP P05556
B	485	GLU	-	expression tag	UNP P05556

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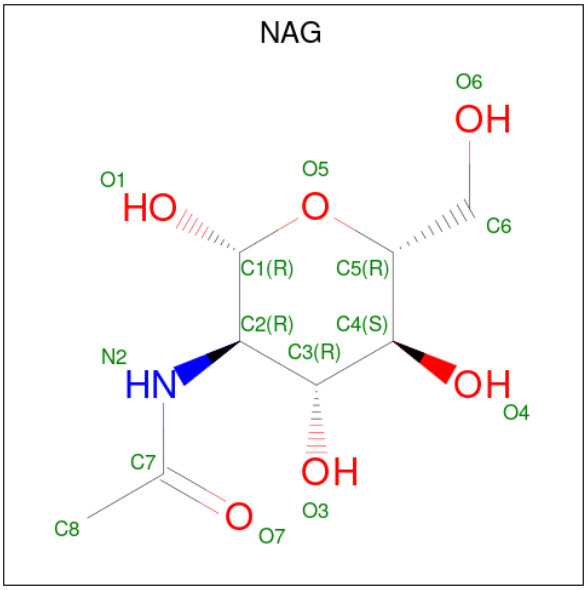
Chain	Residue	Modelled	Actual	Comment	Reference
B	486	ASN	-	expression tag	UNP P05556
B	487	LEU	-	expression tag	UNP P05556
B	488	TYR	-	expression tag	UNP P05556
B	489	PHE	-	expression tag	UNP P05556
B	490	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called Bio-1211.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	D	5	97	36	46	6	9	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0

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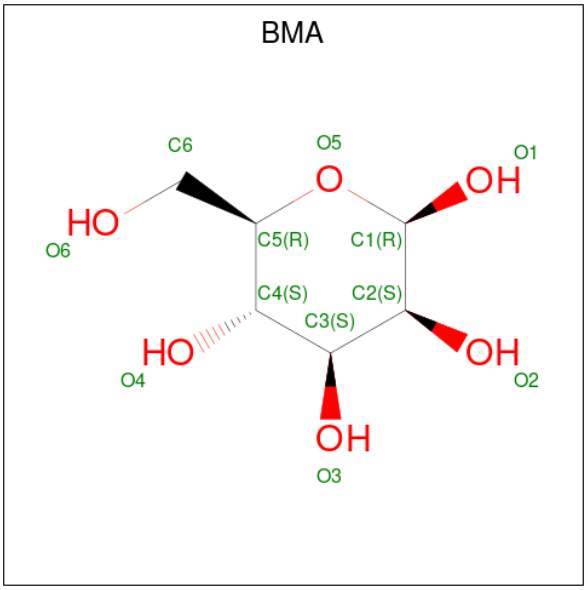
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	A	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	B	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	B	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
4	B	1	28	8	14	1	5	0	0

- Molecule 5 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).

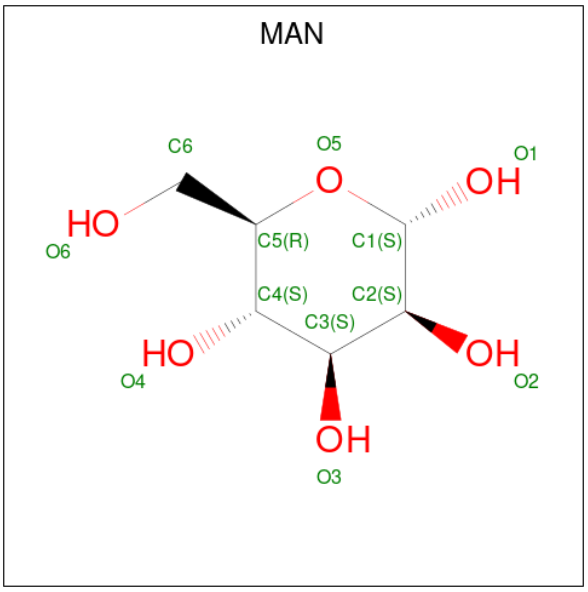


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	22	6	11	5	0	0
			Total	C	H	O		
5	A	1	22	6	11	5	0	0
			Total	C	H	O		
5	A	1	22	6	11	5	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	3	3	3	0	0

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	22	6	11	5	0	0
			Total	C	H	O		
7	A	1	22	6	11	5	0	0
			Total	C	H	O		
7	A	1	22	6	11	5	0	0
			Total	C	H	O		
7	A	1	22	6	11	5	0	0
			Total	C	H	O		
7	A	1	22	6	11	5	0	0

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
8	B	2	2	2	0	0

- Molecule 9 is water.

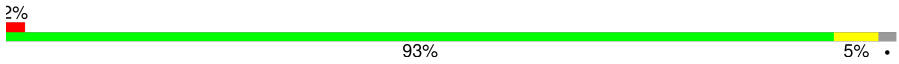
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	3	3	3	0	0
			Total	O		
9	B	2	2	2	0	0

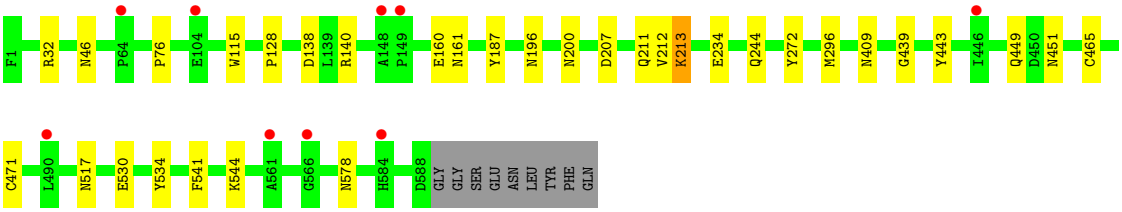
3 Residue-property plots (i)

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: Integrin alpha-4,Integrin alpha-V heavy chain

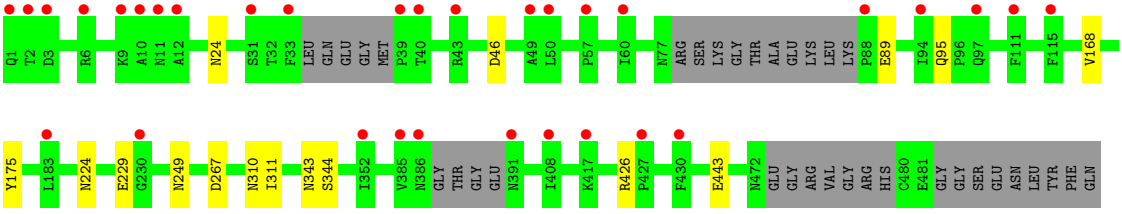
Chain A:





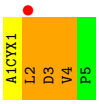
- Molecule 2: Integrin beta-1

Chain B:



- Molecule 3: Bio-1211

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	84.46Å 109.64Å 131.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.51 – 2.64 35.51 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.51-2.64) 98.6 (35.51-2.64)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.253 , 0.290 0.255 , 0.291	Depositor DCC
R_{free} test set	1826 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16491	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: A1CYX, NAG, MAN, MN, BMA, 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	0.11	0/4624	0.30	0/6259
2	B	0.10	0/3565	0.26	0/4816
3	D	3.81	3/31 (9.7%)	1.12	0/41
All	All	0.26	3/8220 (0.0%)	0.29	0/11116

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	ASP	C-N	13.07	1.48	1.33
3	D	2	LEU	C-N	11.17	1.48	1.33
3	D	4	VAL	C-N	8.50	1.48	1.34

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	4531	4439	4439	27	0
2	B	3505	3369	3369	8	0
3	D	51	46	30	6	0
4	A	140	140	130	15	0
4	B	42	42	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	33	33	30	5	0
6	A	3	0	0	0	0
7	A	55	55	50	3	0
8	B	2	0	0	0	0
9	A	3	0	0	0	0
9	B	2	0	0	0	0
All	All	8367	8124	8087	48	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 3.

The worst 5 of 48 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)
4:A:609:NAG:O4	5:A:610:BMA:O2	2.01	0.77
4:A:619:NAG:HO4	5:A:620:BMA:HO2	0.78	0.76
1:A:46:ASN:ND2	1:A:76:PRO:O	2.34	0.60
1:A:439:GLY:O	1:A:471:CYS:N	2.34	0.60
4:A:615:NAG:O4	4:A:617:NAG:O7	2.20	0.60

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	586/597 (98%)	567 (97%)	17 (3%)	2 (0%)	36 50
2	B	445/490 (91%)	428 (96%)	17 (4%)	0	100 100
3	D	2/5 (40%)	2 (100%)	0	0	100 100
All	All	1033/1092 (95%)	997 (96%)	34 (3%)	2 (0%)	43 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	A	161	ASN

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	487/496 (98%)	484 (99%)	3 (1%)	78	87
2	B	399/431 (93%)	395 (99%)	4 (1%)	68	80
3	D	4/4 (100%)	4 (100%)	0	100	100
All	All	890/931 (96%)	883 (99%)	7 (1%)	73	84

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

Mol	Chain	Res	Type
2	B	95	GLN
2	B	224	ASN
2	B	443	GLU
2	B	311	ILE
1	A	578	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
2	B	109	GLN
2	B	343	ASN
2	B	322	GLN
1	A	262	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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	NAG	A	601	-	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	A	609	-	14,14,15	1.06	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	A	608	-	14,14,15	1.25	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	A	603	-	14,14,15	0.67	1 (7%)	17,19,21	0.66	0
7	MAN	A	611	-	11,11,12	0.86	1 (9%)	15,15,17	1.14	2 (13%)
7	MAN	A	613	-	11,11,12	0.71	0	15,15,17	1.18	2 (13%)
5	BMA	A	604	-	11,11,12	0.81	0	15,15,17	0.74	0
4	NAG	A	615	-	14,14,15	0.49	0	17,19,21	0.49	0
4	NAG	A	616	-	14,14,15	0.28	0	17,19,21	0.37	0
4	NAG	B	505	-	14,14,15	0.65	1 (7%)	17,19,21	0.61	0
4	NAG	B	501	-	14,14,15	0.83	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	A	618	-	14,14,15	1.01	1 (7%)	17,19,21	0.65	0
4	NAG	A	619	-	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
7	MAN	A	612	-	11,11,12	0.66	0	15,15,17	1.20	2 (13%)
4	NAG	A	617	-	14,14,15	0.27	0	17,19,21	0.61	0
7	MAN	A	614	-	11,11,12	0.68	0	15,15,17	1.04	1 (6%)
7	MAN	A	621	-	11,11,12	0.80	0	15,15,17	1.05	1 (6%)
5	BMA	A	610	-	11,11,12	0.95	1 (9%)	15,15,17	0.81	0
4	NAG	B	502	-	14,14,15	0.40	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BMA	A	620	-	11,11,12	1.42	2 (18%)	15,15,17	0.89	0
4	NAG	A	602	-	14,14,15	0.77	1 (7%)	17,19,21	0.71	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	A	601	-	-	2/6/23/26	0/1/1/1
4	NAG	A	609	-	-	2/6/23/26	0/1/1/1
4	NAG	A	608	-	-	2/6/23/26	0/1/1/1
4	NAG	A	603	-	-	0/6/23/26	0/1/1/1
7	MAN	A	611	-	-	0/2/19/22	1/1/1/1
7	MAN	A	613	-	-	1/2/19/22	1/1/1/1
5	BMA	A	604	-	-	0/2/19/22	0/1/1/1
4	NAG	A	615	-	-	2/6/23/26	0/1/1/1
4	NAG	A	616	-	-	3/6/23/26	0/1/1/1
4	NAG	B	505	-	-	4/6/23/26	0/1/1/1
4	NAG	B	501	-	-	0/6/23/26	0/1/1/1
4	NAG	A	618	-	-	0/6/23/26	0/1/1/1
4	NAG	A	619	-	-	4/6/23/26	0/1/1/1
7	MAN	A	612	-	-	2/2/19/22	0/1/1/1
4	NAG	A	617	-	-	0/6/23/26	0/1/1/1
7	MAN	A	614	-	-	2/2/19/22	0/1/1/1
7	MAN	A	621	-	-	2/2/19/22	1/1/1/1
5	BMA	A	610	-	-	0/2/19/22	0/1/1/1
4	NAG	B	502	-	-	2/6/23/26	0/1/1/1
5	BMA	A	620	-	-	0/2/19/22	0/1/1/1
4	NAG	A	602	-	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	NAG	O5-C1	-4.19	1.36	1.43
4	A	618	NAG	O5-C1	-3.67	1.37	1.43
5	A	620	BMA	O5-C1	-3.48	1.37	1.43
4	A	609	NAG	O5-C1	-3.38	1.38	1.43
5	A	620	BMA	C4-C5	2.52	1.58	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	613	MAN	C1-O5-C5	3.46	116.82	112.19
7	A	611	MAN	C1-O5-C5	3.42	116.78	112.19
7	A	621	MAN	C1-O5-C5	3.19	116.46	112.19
7	A	612	MAN	C1-O5-C5	2.97	116.17	112.19
4	A	619	NAG	C1-O5-C5	2.59	115.66	112.19

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	616	NAG	C1-C2-N2-C7
4	B	505	NAG	O5-C5-C6-O6
4	A	609	NAG	O5-C5-C6-O6
4	A	619	NAG	C4-C5-C6-O6
4	B	505	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	621	MAN	C1-C2-C3-C4-C5-O5
7	A	611	MAN	C1-C2-C3-C4-C5-O5
7	A	613	MAN	C1-C2-C3-C4-C5-O5

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	609	NAG	3	0
4	A	608	NAG	2	0
4	A	603	NAG	1	0
7	A	613	MAN	1	0
4	A	615	NAG	2	0
4	B	505	NAG	1	0
4	B	501	NAG	2	0
4	A	618	NAG	5	0
4	A	619	NAG	2	0
7	A	612	MAN	2	0
4	A	617	NAG	2	0
7	A	621	MAN	1	0
5	A	610	BMA	3	0
4	B	502	NAG	1	0
5	A	620	BMA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	NAG	3	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	588/597 (98%)	0.15	9 (1%)	72	69	57, 89, 146, 226	0
2	B	455/490 (92%)	0.58	32 (7%)	22	18	59, 121, 182, 241	0
3	D	4/5 (80%)	1.34	1 (25%)	2	1	126, 127, 131, 137	0
All	All	1047/1092 (95%)	0.34	42 (4%)	42	35	57, 100, 167, 241	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	THR	7.7
2	B	385	VAL	5.2
2	B	31	SER	3.8
2	B	3	ASP	3.7
1	A	148	ALA	3.6

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)

There are no oligosaccharides in this entry.

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
5	BMA	A	604	11/12	0.17	0.12	165,168,201,202	0
4	NAG	B	502	14/15	0.18	0.20	139,151,179,181	0
7	MAN	A	621	11/12	0.34	0.14	137,141,169,169	0
5	BMA	A	620	11/12	0.37	0.12	132,137,164,165	0
7	MAN	A	614	11/12	0.42	0.12	132,135,161,162	0
4	NAG	A	616	14/15	0.47	0.12	118,128,152,153	0
4	NAG	A	615	14/15	0.49	0.17	104,120,139,144	0
4	NAG	A	618	14/15	0.54	0.17	124,130,155,157	0
4	NAG	A	603	14/15	0.54	0.13	125,136,161,163	0
4	NAG	B	505	14/15	0.56	0.13	126,130,154,156	0
7	MAN	A	611	11/12	0.56	0.13	97,103,119,124	0
4	NAG	A	619	14/15	0.58	0.14	127,131,156,157	0
7	MAN	A	613	11/12	0.61	0.15	113,118,141,142	0
4	NAG	A	601	14/15	0.65	0.12	107,116,139,139	0
4	NAG	A	608	14/15	0.66	0.20	96,113,135,136	0
7	MAN	A	612	11/12	0.68	0.12	84,90,104,108	0
4	NAG	A	617	14/15	0.69	0.10	124,134,160,161	0
4	NAG	A	609	14/15	0.70	0.14	95,103,124,124	0
4	NAG	B	501	14/15	0.74	0.15	135,139,166,166	0
4	NAG	A	602	14/15	0.80	0.14	104,108,130,130	0
5	BMA	A	610	11/12	0.89	0.10	91,99,117,119	0
6	CA	A	607	1/1	0.99	0.03	59,59,59,59	0
6	CA	A	605	1/1	0.99	0.02	70,70,70,70	0
6	CA	A	606	1/1	0.99	0.03	62,62,62,62	0
8	MN	B	504	1/1	0.99	0.03	72,72,72,72	0
8	MN	B	503	1/1	1.00	0.04	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.