



wwPDB X-ray Structure Validation Summary Report

Apr 22, 2014 – 09:56 AM EDT

PDB ID : 4MMX
Title : Integrin AlphaVBeta3 ectodomain bound to the tenth domain of Fibronectin
Authors : van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on : 2013-09-09
Resolution : 3.32 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

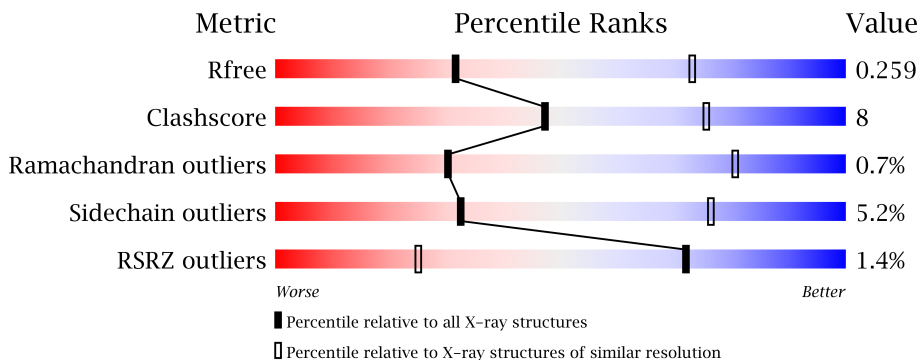
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance




The reported resolution of this entry is 3.32 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}	66092	1372 (3.44-3.20)
Clashscore	79885	1016 (3.42-3.22)
Ramachandran outliers	78287	1699 (3.44-3.20)
Sidechain outliers	78261	1697 (3.44-3.20)
RSRZ outliers	66119	1373 (3.44-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	959	
2	B	692	
3	C	98	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13626 atoms, of which 0 are hydrogen and 0 are deuterium.

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-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	93	Total	C	N	O	0	0	0
			694	438	115	141			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1510	GLY	-	EXPRESSION TAG	UNP P02751
C	1511	LYS	-	EXPRESSION TAG	UNP P02751
C	1512	LYS	-	EXPRESSION TAG	UNP P02751
C	1513	GLY	-	EXPRESSION TAG	UNP P02751
C	1514	LYS	-	EXPRESSION TAG	UNP P02751

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		
4	A	4	Total	C	N	O	0	0
			50	28	2	20		

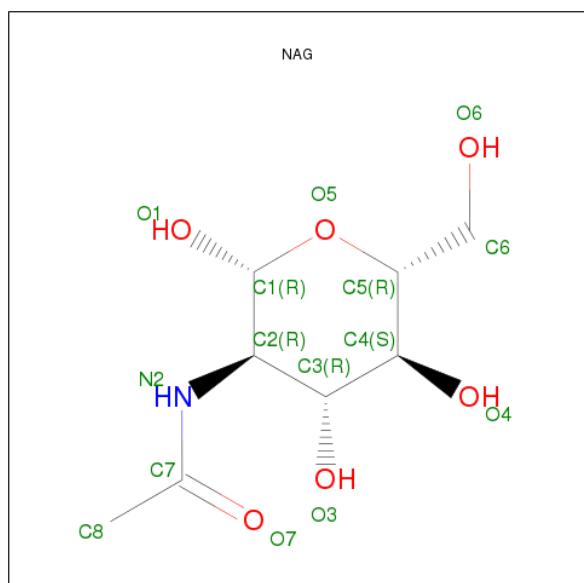
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	3	Total	C	N	O	0	0
			39	22	2	15		
8	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Mn	0	0
			3	3		
9	A	5	Total	Mn	0	0
			5	5		

- Molecule 10 is water.

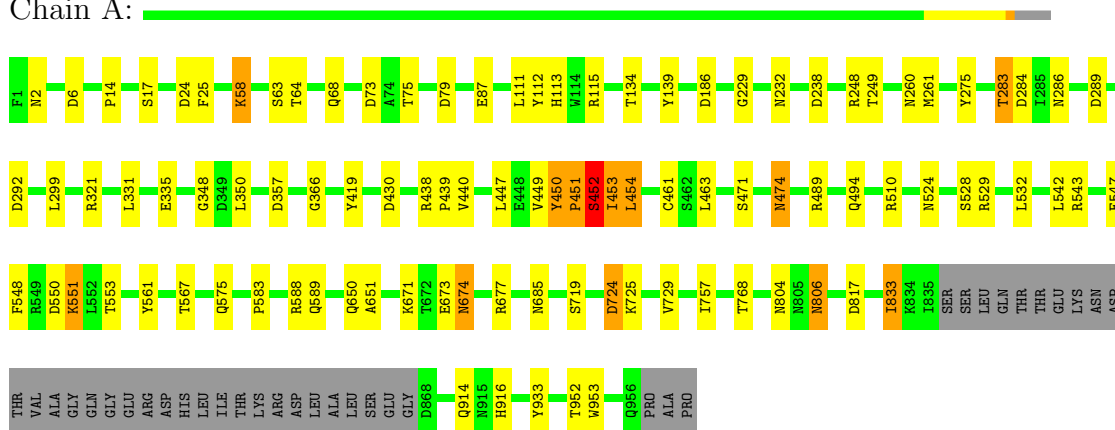
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

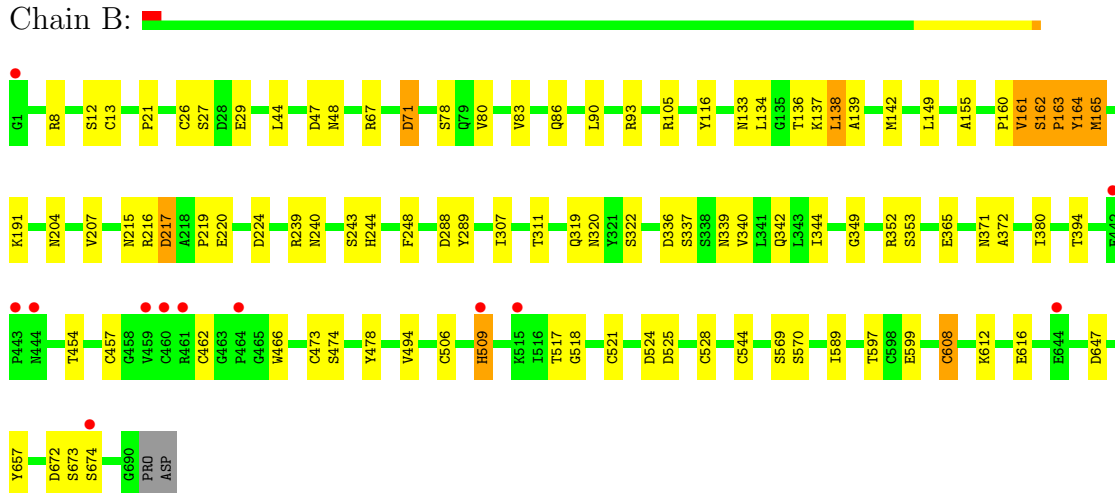
• Molecule 1: Integrin alpha-V

Chain A:



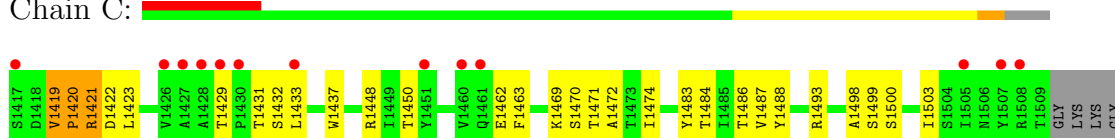
• Molecule 2: Integrin beta-3

Chain B:



• Molecule 3: Fibronectin

Chain C:



LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.86Å 129.86Å 305.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.51 – 3.32 42.51 – 3.32	Depositor EDS
% Data completeness (in resolution range)	88.0 (42.51-3.32) 88.0 (42.51-3.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4.1496)	Depositor
R, R_{free}	0.208 , 0.259 0.208 , 0.259	Depositor DCC
R_{free} test set	1943 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.8	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	26 of 39593 reflections (0.066%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13626	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MN, MAN

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	0.23	0/7352	0.44	1/9967 (0.0%)
2	B	0.26	0/5390	0.48	0/7289
3	C	0.28	0/710	0.57	0/975
All	All	0.24	0/13452	0.46	1/18231 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	TYR	C-N-CD	-8.01	102.97	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7196	0	0	46	0
2	B	5294	0	29	48	0
3	C	694	0	0	14	0
4	A	100	0	86	2	0
5	A	84	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	25	0	0
6	A	72	0	61	2	0
7	A	42	0	39	1	0
7	B	28	0	26	2	0
8	A	39	0	34	0	0
8	B	39	0	34	1	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	B	2	0	0	0	0
All	All	13626	0	409	112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 112 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:162:SER:CB	2:B:163:PRO:CD	2.30	1.08
1:A:454:LEU:CD2	1:A:454:LEU:N	2.30	0.94
1:A:450:TYR:CB	1:A:451:PRO:CD	2.50	0.89
2:B:161:VAL:O	2:B:162:SER:O	1.94	0.84
1:A:449:VAL:O	1:A:449:VAL:CG1	2.30	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	920/959 (96%)	847 (92%)	69 (8%)	4 (0%)	43	89
2	B	688/692 (99%)	597 (87%)	85 (12%)	6 (1%)	25	76
3	C	91/98 (93%)	73 (80%)	16 (18%)	2 (2%)	10	55
All	All	1699/1749 (97%)	1517 (89%)	170 (10%)	12 (1%)	30	80

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	PRO
2	B	162	SER
2	B	163	PRO
1	A	833	ILE
2	B	161	VAL

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	784/813 (96%)	748 (95%)	36 (5%)	37	80
2	B	612/614 (100%)	580 (95%)	32 (5%)	32	76
3	C	78/81 (96%)	69 (88%)	9 (12%)	8	35
All	All	1474/1508 (98%)	1397 (95%)	77 (5%)	32	76

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	916	HIS
2	B	138	LEU
3	C	1469	LYS
1	A	933	TYR
2	B	71	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

28 carbohydrates 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	A	1001	1,4	12,14,15	0.40	0	15,19,21	0.38	0
4	NAG	A	1002	4	12,14,15	0.36	0	15,19,21	0.27	0
4	BMA	A	1003	4	10,11,12	0.78	0	11,15,17	1.29	1 (9%)
4	MAN	A	1004	4	10,11,12	0.38	0	11,15,17	0.82	1 (9%)
5	NAG	A	1005	1,5	12,14,15	0.60	0	15,19,21	1.67	2 (13%)
5	NAG	A	1006	5	12,14,15	0.36	0	15,19,21	0.28	0
6	NAG	A	1007	1,6	12,14,15	0.37	0	15,19,21	0.31	0
6	NAG	A	1008	6	12,14,15	0.38	0	15,19,21	0.30	0
6	BMA	A	1009	6	10,11,12	0.63	0	11,15,17	0.83	0
6	MAN	A	1010	6	10,11,12	0.44	0	11,15,17	0.94	1 (9%)
6	BMA	A	1011	6	10,11,12	1.03	1 (10%)	11,15,17	1.29	1 (9%)
6	MAN	A	1012	6	10,11,12	0.66	0	11,15,17	1.19	2 (18%)
4	NAG	A	1013	1,4	12,14,15	0.36	0	15,19,21	0.30	0
4	NAG	A	1014	4	12,14,15	0.38	0	15,19,21	0.30	0
4	BMA	A	1015	4	10,11,12	0.59	0	11,15,17	0.91	0
4	MAN	A	1016	4	10,11,12	0.43	0	11,15,17	0.90	1 (9%)
5	NAG	A	1018	1,5	12,14,15	0.35	0	15,19,21	0.30	0
5	NAG	A	1019	5	12,14,15	0.37	0	15,19,21	0.28	0
5	NAG	A	1022	1,5	12,14,15	0.38	0	15,19,21	0.30	0
5	NAG	A	1023	5	12,14,15	0.32	0	15,19,21	0.22	0
8	NAG	A	1024	1,8	12,14,15	0.41	0	15,19,21	0.35	0
8	NAG	A	1025	8	12,14,15	0.37	0	15,19,21	0.34	0
8	BMA	A	1026	8	10,11,12	0.70	0	11,15,17	1.40	2 (18%)
5	NAG	B	703	2,5	12,14,15	0.36	0	15,19,21	0.68	0
5	NAG	B	704	5	12,14,15	0.34	0	15,19,21	0.58	0
8	NAG	B	705	8,2	12,14,15	0.36	0	15,19,21	0.27	0
8	NAG	B	706	8	12,14,15	0.31	0	15,19,21	0.38	0
8	BMA	B	707	8	10,11,12	0.52	0	11,15,17	1.07	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	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1006	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1007	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1008	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1009	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1010	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1011	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1012	6	-	0/2/19/22	0/1/1/1
4	NAG	A	1013	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1015	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1016	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1018	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1019	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1022	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1023	5	-	0/6/23/26	0/1/1/1
8	NAG	A	1024	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1025	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1026	8	-	0/2/19/22	0/1/1/1
5	NAG	B	703	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	704	5	-	0/6/23/26	0/1/1/1
8	NAG	B	705	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	706	8	-	0/6/23/26	0/1/1/1
8	BMA	B	707	8	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1011	BMA	C4-C5	2.19	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1005	NAG	C2-N2-C7	5.06	129.51	123.39
8	A	1026	BMA	O5-C5-C4	-3.24	106.54	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1005	NAG	C3-C4-C5	3.16	115.84	110.17
4	A	1003	BMA	O3-C3-C2	3.07	115.32	109.74
6	A	1011	BMA	C4-C3-C2	2.49	113.39	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
7	NAG	A	1017	1	12,14,15	0.35	0	15,19,21	0.30	0
7	NAG	A	1020	1	12,14,15	0.29	0	15,19,21	0.31	0
7	NAG	A	1021	1	12,14,15	0.35	0	15,19,21	0.29	0
7	NAG	B	701	2	12,14,15	0.30	0	15,19,21	0.34	0
7	NAG	B	702	2	12,14,15	0.39	0	15,19,21	0.37	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	A	1017	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1020	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	924/959 (96%)	-0.10	0 100 100	42, 87, 140, 175	0
2	B	690/692 (99%)	0.04	12 (1%) 67 21	49, 102, 207, 251	1 (0%)
3	C	93/98 (94%)	1.01	13 (13%) 3 1	74, 188, 325, 345	0
All	All	1707/1749 (97%)	0.02	25 (1%) 72 24	42, 95, 198, 345	1 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1428	ALA	7.1
2	B	443	PRO	5.4
2	B	460	CYS	4.4
3	C	1426	VAL	4.2
3	C	1427	ALA	4.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	1002	14/15	0.23	30.00	103,115,120,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	1022	14/15	0.20	1.28	97,118,133,136	0
5	NAG	B	704	14/15	0.22	0.70	140,144,159,165	0
5	NAG	A	1005	14/15	0.23	0.65	96,114,123,131	0
4	NAG	A	1014	14/15	0.30	0.33	123,139,153,160	0
5	NAG	B	703	14/15	0.20	0.21	91,117,137,142	0
4	NAG	A	1001	14/15	0.17	-0.31	66,76,92,96	0
4	NAG	A	1013	14/15	0.20	-0.49	92,110,124,132	0
4	MAN	A	1016	11/12	0.26	-0.93	161,170,176,179	0
8	NAG	B	706	14/15	0.20	-0.94	93,108,120,120	0
8	NAG	B	705	14/15	0.13	-1.04	61,87,93,93	0
6	NAG	A	1008	14/15	0.15	-1.25	44,60,84,91	0
6	MAN	A	1012	11/12	0.20	-1.25	103,110,119,120	0
6	NAG	A	1007	14/15	0.12	-1.29	40,54,83,85	0
5	NAG	A	1018	14/15	0.15	-1.47	101,117,128,132	0
8	BMA	B	707	11/12	0.15	-1.60	100,109,116,117	0
6	BMA	A	1011	11/12	0.15	-1.85	92,107,128,129	0
8	NAG	A	1024	14/15	0.12	-2.55	64,88,106,108	0
4	BMA	A	1015	11/12	0.43	-	156,158,170,178	0
8	BMA	A	1026	11/12	0.42	-	175,181,190,190	0
5	NAG	A	1019	14/15	0.18	-	123,132,135,138	0
4	MAN	A	1004	11/12	0.51	-	164,172,177,180	0
6	MAN	A	1010	11/12	0.22	-	114,126,140,141	0
5	NAG	A	1023	14/15	0.36	-	141,148,157,159	0
8	NAG	A	1025	14/15	0.40	-	129,145,164,177	0
4	BMA	A	1003	11/12	0.41	-	148,158,162,169	0
6	BMA	A	1009	11/12	0.11	-	93,100,116,127	0
5	NAG	A	1006	14/15	0.32	-	125,134,144,148	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	A	1021	14/15	0.21	1.81	92,108,117,120	0
7	NAG	B	701	14/15	0.27	0.87	99,127,136,146	0
9	MN	B	709	1/1	0.20	0.22	88,88,88,88	0
7	NAG	A	1017	14/15	0.21	-0.19	124,142,149,152	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MN	A	1031	1/1	0.11	-0.28	84,84,84,84	0
9	MN	A	1029	1/1	0.15	-0.44	177,177,177,177	0
9	MN	B	710	1/1	0.22	-0.65	56,56,56,56	0
9	MN	A	1028	1/1	0.12	-0.77	90,90,90,90	0
9	MN	A	1030	1/1	0.16	-0.99	137,137,137,137	0
7	NAG	B	702	14/15	0.16	-1.10	80,95,106,114	0
9	MN	A	1027	1/1	0.08	-1.26	89,89,89,89	0
9	MN	B	708	1/1	0.17	-1.65	48,48,48,48	0
7	NAG	A	1020	14/15	0.35	-	136,151,158,158	0

6.5 Other polymers ⓘ

There are no such residues in this entry.