



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 05:11 PM BST

PDB ID : 5N6U
Title : Crystal structure of Beta-D-Mannosidase from Dictyoglomus thermophilum.
Authors : Richet, N.; Lafite, P.
Deposited on : 2017-02-16
Resolution : 3.08 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

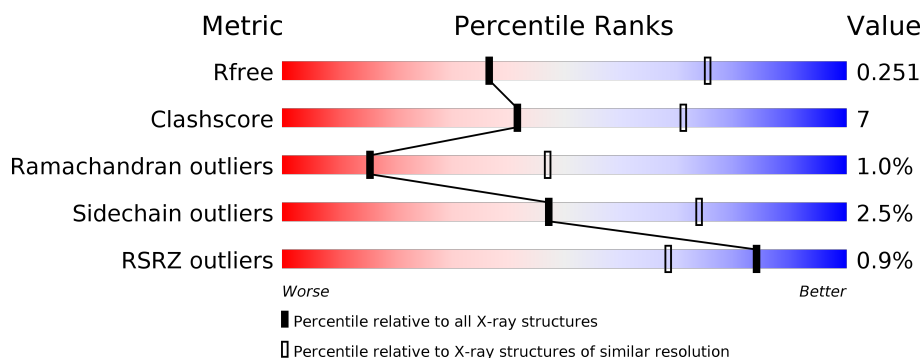
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 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	836	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 80%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 15% • • </div> </div>
1	B	836	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 79%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 17% • • </div> </div>
1	C	836	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 18% • • </div> </div>
1	D	836	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 79%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 15% • • </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27265 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 Beta-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	B	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	C	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	D	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP B5YAN4
A	-21	GLY	-	expression tag	UNP B5YAN4
A	-20	SER	-	expression tag	UNP B5YAN4
A	-19	SER	-	expression tag	UNP B5YAN4
A	-18	HIS	-	expression tag	UNP B5YAN4
A	-17	HIS	-	expression tag	UNP B5YAN4
A	-16	HIS	-	expression tag	UNP B5YAN4
A	-15	HIS	-	expression tag	UNP B5YAN4
A	-14	HIS	-	expression tag	UNP B5YAN4
A	-13	HIS	-	expression tag	UNP B5YAN4
A	-12	SER	-	expression tag	UNP B5YAN4
A	-11	SER	-	expression tag	UNP B5YAN4
A	-10	GLY	-	expression tag	UNP B5YAN4
A	-9	LEU	-	expression tag	UNP B5YAN4
A	-8	VAL	-	expression tag	UNP B5YAN4
A	-7	PRO	-	expression tag	UNP B5YAN4
A	-6	ARG	-	expression tag	UNP B5YAN4
A	-5	GLY	-	expression tag	UNP B5YAN4
A	-4	SER	-	expression tag	UNP B5YAN4
A	-3	HIS	-	expression tag	UNP B5YAN4
A	-2	MET	-	expression tag	UNP B5YAN4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP B5YAN4
A	0	SER	-	expression tag	UNP B5YAN4
A	425	CYS	GLU	engineered mutation	UNP B5YAN4
B	-22	MET	-	initiating methionine	UNP B5YAN4
B	-21	GLY	-	expression tag	UNP B5YAN4
B	-20	SER	-	expression tag	UNP B5YAN4
B	-19	SER	-	expression tag	UNP B5YAN4
B	-18	HIS	-	expression tag	UNP B5YAN4
B	-17	HIS	-	expression tag	UNP B5YAN4
B	-16	HIS	-	expression tag	UNP B5YAN4
B	-15	HIS	-	expression tag	UNP B5YAN4
B	-14	HIS	-	expression tag	UNP B5YAN4
B	-13	HIS	-	expression tag	UNP B5YAN4
B	-12	SER	-	expression tag	UNP B5YAN4
B	-11	SER	-	expression tag	UNP B5YAN4
B	-10	GLY	-	expression tag	UNP B5YAN4
B	-9	LEU	-	expression tag	UNP B5YAN4
B	-8	VAL	-	expression tag	UNP B5YAN4
B	-7	PRO	-	expression tag	UNP B5YAN4
B	-6	ARG	-	expression tag	UNP B5YAN4
B	-5	GLY	-	expression tag	UNP B5YAN4
B	-4	SER	-	expression tag	UNP B5YAN4
B	-3	HIS	-	expression tag	UNP B5YAN4
B	-2	MET	-	expression tag	UNP B5YAN4
B	-1	ALA	-	expression tag	UNP B5YAN4
B	0	SER	-	expression tag	UNP B5YAN4
B	425	CYS	GLU	engineered mutation	UNP B5YAN4
C	-22	MET	-	initiating methionine	UNP B5YAN4
C	-21	GLY	-	expression tag	UNP B5YAN4
C	-20	SER	-	expression tag	UNP B5YAN4
C	-19	SER	-	expression tag	UNP B5YAN4
C	-18	HIS	-	expression tag	UNP B5YAN4
C	-17	HIS	-	expression tag	UNP B5YAN4
C	-16	HIS	-	expression tag	UNP B5YAN4
C	-15	HIS	-	expression tag	UNP B5YAN4
C	-14	HIS	-	expression tag	UNP B5YAN4
C	-13	HIS	-	expression tag	UNP B5YAN4
C	-12	SER	-	expression tag	UNP B5YAN4
C	-11	SER	-	expression tag	UNP B5YAN4
C	-10	GLY	-	expression tag	UNP B5YAN4
C	-9	LEU	-	expression tag	UNP B5YAN4
C	-8	VAL	-	expression tag	UNP B5YAN4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP B5YAN4
C	-6	ARG	-	expression tag	UNP B5YAN4
C	-5	GLY	-	expression tag	UNP B5YAN4
C	-4	SER	-	expression tag	UNP B5YAN4
C	-3	HIS	-	expression tag	UNP B5YAN4
C	-2	MET	-	expression tag	UNP B5YAN4
C	-1	ALA	-	expression tag	UNP B5YAN4
C	0	SER	-	expression tag	UNP B5YAN4
C	425	CYS	GLU	engineered mutation	UNP B5YAN4
D	-22	MET	-	initiating methionine	UNP B5YAN4
D	-21	GLY	-	expression tag	UNP B5YAN4
D	-20	SER	-	expression tag	UNP B5YAN4
D	-19	SER	-	expression tag	UNP B5YAN4
D	-18	HIS	-	expression tag	UNP B5YAN4
D	-17	HIS	-	expression tag	UNP B5YAN4
D	-16	HIS	-	expression tag	UNP B5YAN4
D	-15	HIS	-	expression tag	UNP B5YAN4
D	-14	HIS	-	expression tag	UNP B5YAN4
D	-13	HIS	-	expression tag	UNP B5YAN4
D	-12	SER	-	expression tag	UNP B5YAN4
D	-11	SER	-	expression tag	UNP B5YAN4
D	-10	GLY	-	expression tag	UNP B5YAN4
D	-9	LEU	-	expression tag	UNP B5YAN4
D	-8	VAL	-	expression tag	UNP B5YAN4
D	-7	PRO	-	expression tag	UNP B5YAN4
D	-6	ARG	-	expression tag	UNP B5YAN4
D	-5	GLY	-	expression tag	UNP B5YAN4
D	-4	SER	-	expression tag	UNP B5YAN4
D	-3	HIS	-	expression tag	UNP B5YAN4
D	-2	MET	-	expression tag	UNP B5YAN4
D	-1	ALA	-	expression tag	UNP B5YAN4
D	0	SER	-	expression tag	UNP B5YAN4
D	425	CYS	GLU	engineered mutation	UNP B5YAN4

- Molecule 2 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

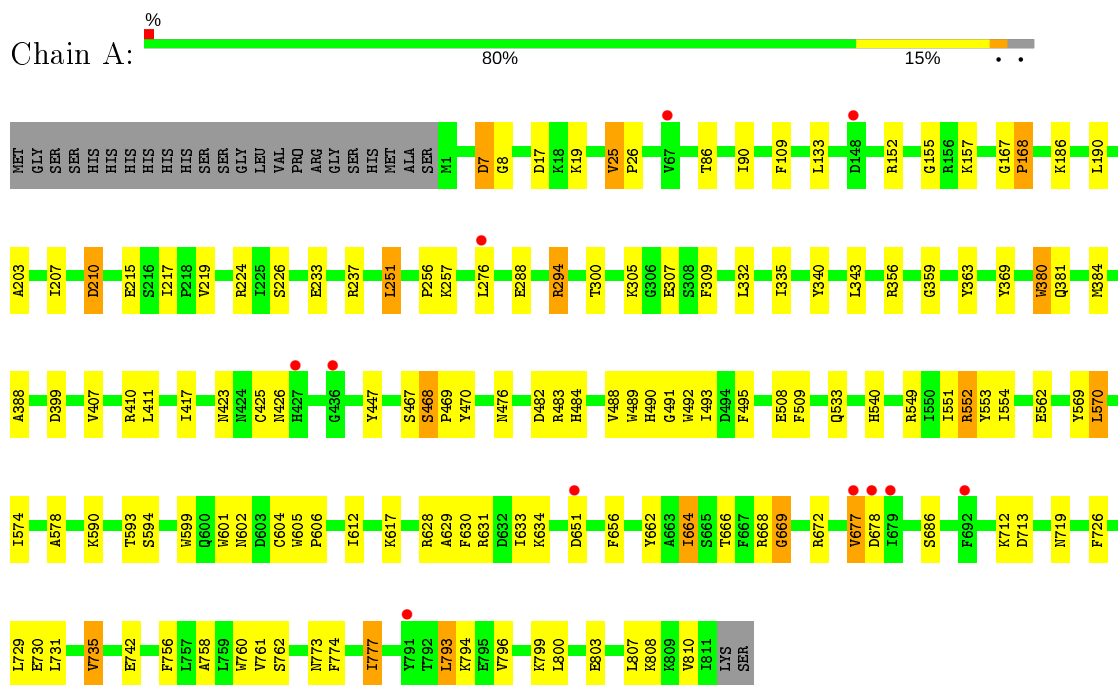
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	4	Total	O	0	0
			4	4		
3	C	10	Total	O	0	0
			10	10		
3	D	5	Total	O	0	0
			5	5		

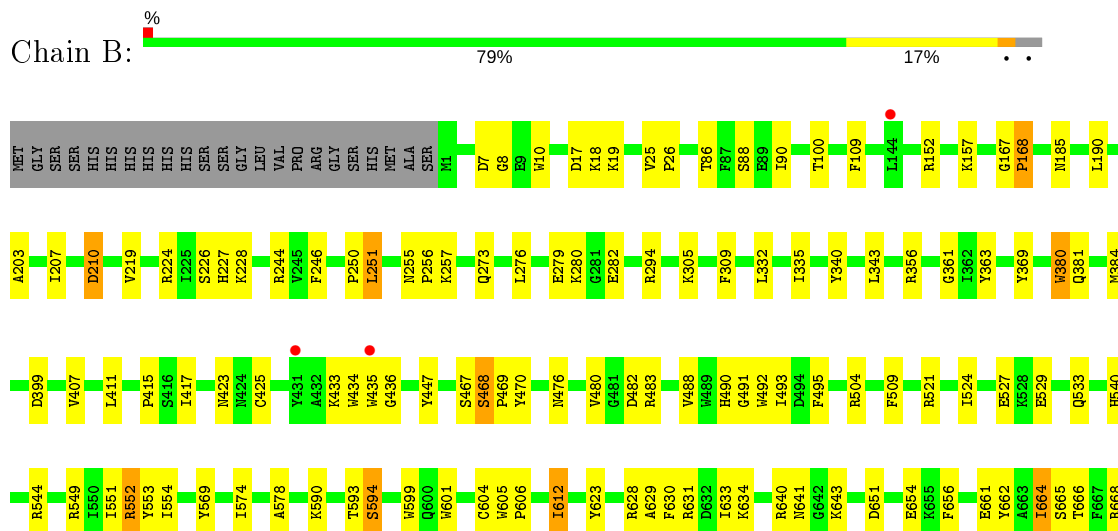
3 Residue-property plots

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: Beta-mannosidase



- Molecule 1: Beta-mannosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.25Å 75.56Å 217.88Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	49.50 – 3.08 48.48 – 3.19	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.50-3.08) 98.9 (48.48-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.204 , 0.255 0.203 , 0.251	Depositor DCC
R_{free} test set	3775 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
Reported twinning fraction	0.913 for H, K, L 0.087 for -h,-k,l	Depositor
Outliers	4 of 75507 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27265	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: BMA

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	0/6995	0.86	10/9461 (0.1%)
1	B	0.60	0/6995	0.89	13/9461 (0.1%)
1	C	0.61	1/6995 (0.0%)	0.90	16/9461 (0.2%)
1	D	0.62	0/6995	0.91	18/9461 (0.2%)
All	All	0.60	1/27980 (0.0%)	0.89	57/37844 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	4
1	D	0	6
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	599	TRP	CG-CD1	6.09	1.45	1.36

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	C	334	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	C	802	LEU	CA-CB-CG	9.51	137.17	115.30
1	B	552	ARG	NE-CZ-NH1	-8.93	115.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	552	ARG	NE-CZ-NH2	8.49	124.54	120.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	VAL	Peptide
1	A	257	LYS	Peptide
1	A	468	SER	Peptide
1	A	669	GLY	Peptide
1	A	713	ASP	Peptide

5.2 Too-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 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	6800	0	6675	87	1
1	B	6800	0	6675	89	2
1	C	6800	0	6675	112	10
1	D	6800	0	6675	99	2
2	A	11	0	10	0	0
2	B	11	0	10	0	0
2	C	11	0	10	0	0
2	D	11	0	10	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	27265	0	26740	378	13

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 7.

The worst 5 of 378 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:C:305:LYS:HE2	1:C:592:HIS:CE1	1.85	1.11
1:B:590:LYS:NZ	1:B:651:ASP:OD1	2.01	0.94
1:A:590:LYS:NZ	1:A:651:ASP:OD1	2.01	0.94
1:C:600:GLN:HG3	1:C:610:TRP:O	1.66	0.94
1:D:590:LYS:NZ	1:D:651:ASP:OD1	2.02	0.93

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:NZ	1:C:711:GLU:C[1_545]	0.73	1.47
1:C:16:LYS:CE	1:C:711:GLU:C[1_545]	1.10	1.10
1:C:16:LYS:NZ	1:C:712:LYS:N[1_545]	1.17	1.03
1:C:16:LYS:CE	1:C:711:GLU:O[1_545]	1.39	0.81
1:C:16:LYS:CE	1:C:712:LYS:N[1_545]	1.47	0.73

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	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	15	47
1	B	809/836 (97%)	715 (88%)	86 (11%)	8 (1%)	15	47
1	C	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	15	47
1	D	809/836 (97%)	725 (90%)	76 (9%)	8 (1%)	15	47
All	All	3236/3344 (97%)	2886 (89%)	318 (10%)	32 (1%)	15	47

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	664	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	152	ARG
1	B	664	ILE
1	B	730	GLU

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	727/748 (97%)	711 (98%)	16 (2%)	52	76
1	B	727/748 (97%)	709 (98%)	18 (2%)	47	74
1	C	727/748 (97%)	707 (97%)	20 (3%)	43	71
1	D	727/748 (97%)	708 (97%)	19 (3%)	46	72
All	All	2908/2992 (97%)	2835 (98%)	73 (2%)	47	74

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	810	VAL
1	C	425	CYS
1	D	662	TYR
1	C	251	LEU
1	C	533	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	589	ASN
1	C	381	GLN
1	D	502	ASN
1	C	314	ASN
1	C	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BMA	B	901	-	11,11,12	2.89	5 (45%)	15,15,17	2.40	3 (20%)
2	BMA	C	901	-	11,11,12	1.68	4 (36%)	15,15,17	1.42	3 (20%)
2	BMA	A	901	-	11,11,12	2.14	5 (45%)	15,15,17	1.57	3 (20%)
2	BMA	D	901	-	11,11,12	2.09	3 (27%)	15,15,17	1.89	3 (20%)

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
2	BMA	B	901	-	-	2/2/19/22	0/1/1/1
2	BMA	C	901	-	-	2/2/19/22	0/1/1/1
2	BMA	A	901	-	-	2/2/19/22	0/1/1/1
2	BMA	D	901	-	-	0/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	BMA	O5-C1	6.99	1.54	1.43
2	A	901	BMA	C2-C3	4.59	1.59	1.52
2	D	901	BMA	C2-C3	4.39	1.59	1.52
2	B	901	BMA	C2-C3	3.95	1.58	1.52
2	D	901	BMA	O5-C1	3.72	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	BMA	O5-C5-C6	7.94	119.66	107.20
2	D	901	BMA	O5-C5-C6	5.05	115.12	107.20
2	A	901	BMA	O5-C5-C6	3.56	112.78	107.20
2	A	901	BMA	C1-O5-C5	3.26	116.61	112.19
2	C	901	BMA	O6-C6-C5	-3.11	100.64	111.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	BMA	O5-C5-C6-O6
2	B	901	BMA	C4-C5-C6-O6
2	A	901	BMA	O5-C5-C6-O6
2	A	901	BMA	C4-C5-C6-O6
2	C	901	BMA	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	811/836 (97%)	0.08	11 (1%) 75 55	53, 86, 130, 161	1 (0%)
1	B	811/836 (97%)	0.02	6 (0%) 87 74	45, 81, 124, 160	1 (0%)
1	C	811/836 (97%)	0.08	9 (1%) 80 63	46, 86, 127, 181	1 (0%)
1	D	811/836 (97%)	0.01	3 (0%) 92 84	47, 82, 123, 175	1 (0%)
All	All	3244/3344 (97%)	0.05	29 (0%) 84 68	45, 84, 126, 181	4 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	PRO	4.5
1	C	695	GLU	3.7
1	D	678	ASP	3.7
1	C	287	VAL	3.7
1	B	435	TRP	3.4

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 monosaccharides 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(\AA^2)	Q<0.9
2	BMA	B	901	11/12	0.86	0.23	58,69,79,82	0
2	BMA	D	901	11/12	0.86	0.24	75,94,105,123	0
2	BMA	C	901	11/12	0.88	0.35	87,103,115,116	0
2	BMA	A	901	11/12	0.91	0.27	71,87,95,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.