



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:19 PM GMT

PDB ID : 1J4U
Title : Structure of Artocarpin Complexed with Me-alpha-Mannose
Authors : Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on : 2001-10-30
Resolution : 2.90 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>

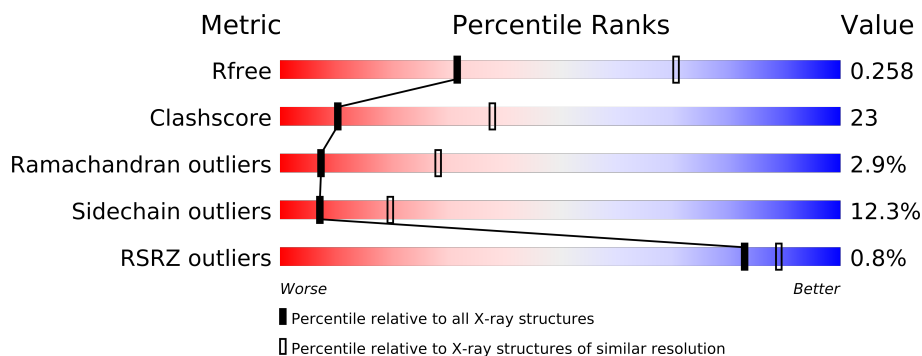
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	149	
1	B	149	
1	C	149	
1	D	149	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4712 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 Artocarpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1133	727	182	223	1			
1	B	149	Total	C	N	O	S	0	0	0
			1133	727	182	223	1			
1	C	149	Total	C	N	O	S	0	0	0
			1133	727	182	223	1			
1	D	149	Total	C	N	O	S	0	0	0
			1133	727	182	223	1			

There are 32 discrepancies between the modelled and reference sequences:

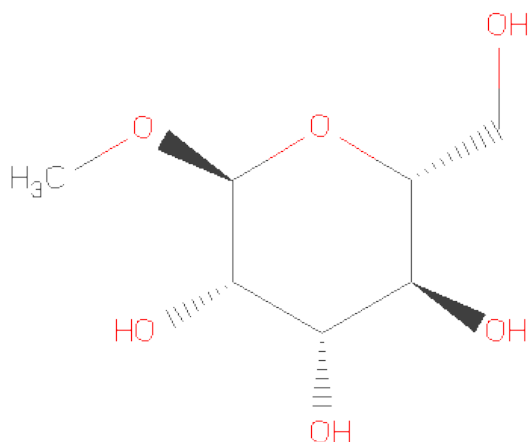
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
A	9	SER	PRO	CONFLICT	UNP Q7M1T4
A	20	GLU	ASP	CONFLICT	UNP Q7M1T4
A	49	ASP	GLU	CONFLICT	UNP Q7M1T4
A	70	LYS	ARG	CONFLICT	UNP Q7M1T4
A	84	GLY	ALA	CONFLICT	UNP Q7M1T4
A	145	ILE	VAL	CONFLICT	UNP Q7M1T4
A	148	SER	ALA	CONFLICT	UNP Q7M1T4
B	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
B	9	SER	PRO	CONFLICT	UNP Q7M1T4
B	20	GLU	ASP	CONFLICT	UNP Q7M1T4
B	49	ASP	GLU	CONFLICT	UNP Q7M1T4
B	70	LYS	ARG	CONFLICT	UNP Q7M1T4
B	84	GLY	ALA	CONFLICT	UNP Q7M1T4
B	145	ILE	VAL	CONFLICT	UNP Q7M1T4
B	148	SER	ALA	CONFLICT	UNP Q7M1T4
C	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
C	9	SER	PRO	CONFLICT	UNP Q7M1T4
C	20	GLU	ASP	CONFLICT	UNP Q7M1T4
C	49	ASP	GLU	CONFLICT	UNP Q7M1T4
C	70	LYS	ARG	CONFLICT	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	84	GLY	ALA	CONFLICT	UNP Q7M1T4
C	145	ILE	VAL	CONFLICT	UNP Q7M1T4
C	148	SER	ALA	CONFLICT	UNP Q7M1T4
D	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
D	9	SER	PRO	CONFLICT	UNP Q7M1T4
D	20	GLU	ASP	CONFLICT	UNP Q7M1T4
D	49	ASP	GLU	CONFLICT	UNP Q7M1T4
D	70	LYS	ARG	CONFLICT	UNP Q7M1T4
D	84	GLY	ALA	CONFLICT	UNP Q7M1T4
D	145	ILE	VAL	CONFLICT	UNP Q7M1T4
D	148	SER	ALA	CONFLICT	UNP Q7M1T4

- Molecule 2 is SUGAR (O1-METHYL-MANNOSE) (three-letter code: MMA) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	C	1	Total	C	O	0	0
			13	7	6		
2	D	1	Total	C	O	0	0
			13	7	6		

- Molecule 3 is water.

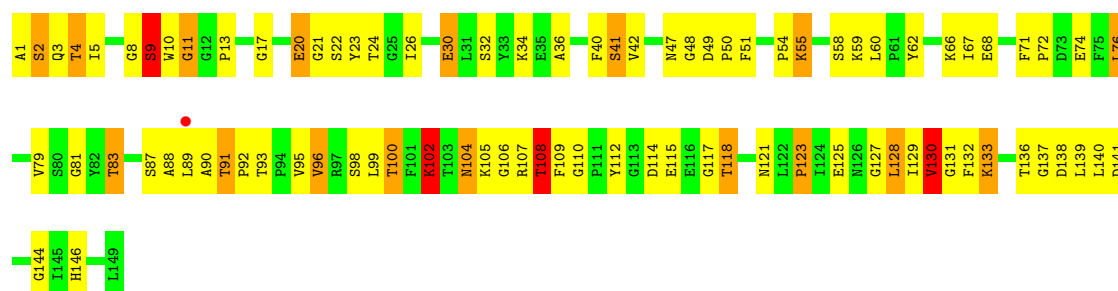
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	33	Total 33	O 33	0	0
3	C	24	Total 24	O 24	0	0
3	D	20	Total 20	O 20	0	0

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.

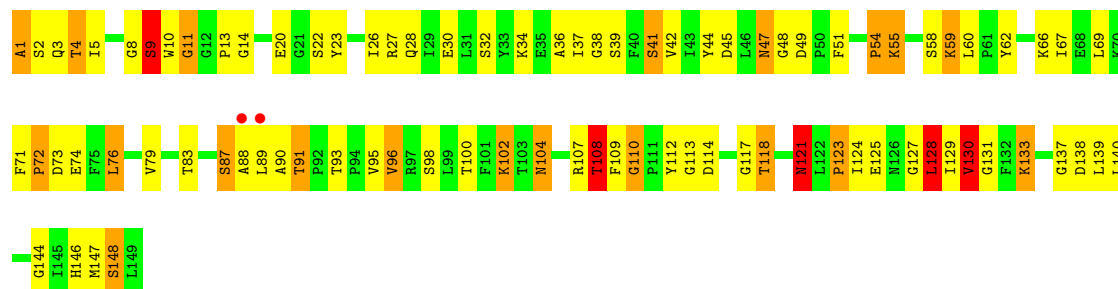
• Molecule 1: Artocarpin

Chain A: 



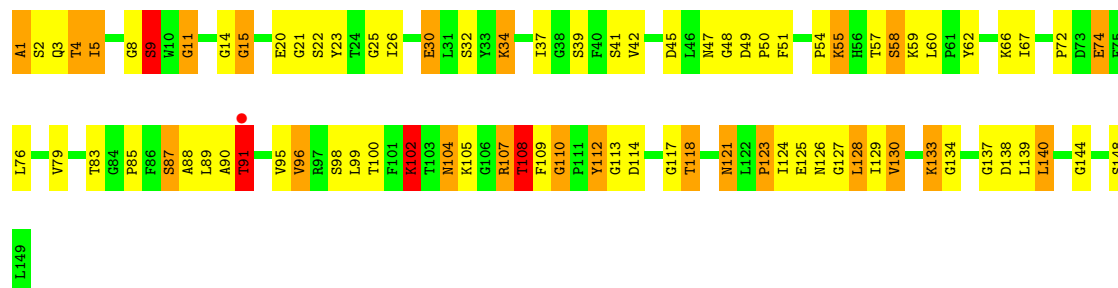
• Molecule 1: Artocarpin

Chain B: 



• Molecule 1: Artocarpin

Chain C: 



• Molecule 1: Artocarpin

L139	L69	A1
L140	K70	Q2
D141	F71	S3
	D72	T4
G144	D73	I5
	E74	T6
M147	F75	V7
S148	L76	G8
L149		S9
	T83	W10
	S87	G11
	A88	G12
	L89	P13
	A90	N16
	T91	G17
	P92	M18
	T93	D19
	P94	E20
	V95	G21
	V96	S22
	R97	Y23
	S98	T24
	L99	G25
	T100	I26
	F101	E30
	K102	
	T103	K34
	N104	E35
	K105	A36
	G106	I37
	T107	G38
	T108	S39
	F109	F40
	G110	S41
	P111	V42
	Y112	
	G113	D45
	D114	L46
	G117	M47
	T118	G48
		D49
	N121	P50
	L122	F51
	P123	S52
	I124	G53
	E125	P54
	N126	K55
	G127	
	L128	S58
	T129	K59
	V130	L60
	G131	F61
	F132	Y62
	K133	G63
	G134	
	G137	K66
	P138	L67
		E68

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	129.20Å 129.20Å 78.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.47 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 90.1 (19.47-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.88Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.258 0.222 , 0.258	Depositor DCC
R_{free} test set	1192 reflections (7.95%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.4	EDS
Estimated twinning fraction	0.070 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 15000 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: AYA, MMA

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	0.46	0/1156	1.93	44/1569 (2.8%)
1	B	0.48	0/1156	1.81	43/1569 (2.7%)
1	C	0.46	0/1156	1.78	43/1569 (2.7%)
1	D	0.47	0/1156	1.79	41/1569 (2.6%)
All	All	0.47	0/4624	1.83	171/6276 (2.7%)

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	1	2
1	B	1	1
1	C	1	1
1	D	0	1
All	All	3	5

There are no bond length outliers.

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	O-C-N	-22.73	86.34	122.70
1	A	2	SER	N-CA-CB	19.20	139.30	110.50
1	B	2	SER	O-C-N	-8.03	109.85	122.70
1	B	2	SER	CB-CA-C	-7.67	95.53	110.10
1	D	2	SER	O-C-N	-7.59	110.56	122.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA
1	C	1	AYA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	AYA	Mainchain
1	A	2	SER	Mainchain
1	B	1	AYA	Mainchain
1	C	1	AYA	Mainchain
1	D	1	AYA	Mainchain

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	1133	0	1084	62	1
1	B	1133	0	1085	63	0
1	C	1133	0	1084	57	0
1	D	1133	0	1085	57	1
2	A	13	0	14	0	0
2	B	13	0	14	0	0
2	C	13	0	14	0	0
2	D	13	0	14	0	0
3	A	51	0	0	12	0
3	B	33	0	0	2	0
3	C	24	0	0	1	0
3	D	20	0	0	1	0
All	All	4712	0	4394	210	1

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 23.

The worst 5 of 210 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:89:LEU:O	1:C:91:THR:HG22	1.58	1.01
1:D:89:LEU:O	1:D:91:THR:HG22	1.60	1.00
1:A:89:LEU:O	1:A:91:THR:HG22	1.61	0.99
1:B:89:LEU:O	1:B:91:THR:HG22	1.65	0.95
1:C:107:ARG:HD2	3:C:270:HOH:O	1.74	0.86

All (1) 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	Distance(Å)	Clash(Å)
1:A:92:PRO:O	1:D:16:ASN:OD1[3_665]	2.10	0.10

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	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	8	30
1	B	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	8	30
1	C	147/149 (99%)	133 (90%)	9 (6%)	5 (3%)	6	23
1	D	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	8	30
All	All	588/596 (99%)	528 (90%)	43 (7%)	17 (3%)	7	28

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	90	ALA
1	A	110	GLY
1	B	9	SER
1	B	90	ALA

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	120/122 (98%)	106 (88%)	14 (12%)	8	22
1	B	120/122 (98%)	105 (88%)	15 (12%)	7	19
1	C	120/122 (98%)	105 (88%)	15 (12%)	7	19
1	D	120/122 (98%)	105 (88%)	15 (12%)	7	19
All	All	480/488 (98%)	421 (88%)	59 (12%)	7	20

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	C	76	LEU
1	D	108	THR
1	B	128	LEU
1	C	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	47	ASN
1	B	104	ASN
1	D	16	ASN
1	B	28	GLN
1	C	104	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	AYA	A	1	1	7,7,8	6.18	3 (42%)	6,8,10	31.36	3 (50%)
1	AYA	B	1	1	7,7,8	7.36	1 (14%)	6,8,10	29.73	3 (50%)
1	AYA	C	1	1	7,7,8	6.31	1 (14%)	6,8,10	32.16	3 (50%)
1	AYA	D	1	1	7,7,8	5.88	3 (42%)	6,8,10	31.06	3 (50%)

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
1	AYA	A	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	B	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	C	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	D	1	1	-	0/4/6/8	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	AYA	O-C	19.31	1.24	1.11
1	C	1	AYA	O-C	16.52	1.22	1.11
1	A	1	AYA	O-C	15.89	1.22	1.11
1	D	1	AYA	O-C	15.12	1.21	1.11
1	A	1	AYA	CA-N	3.10	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	AYA	CB-CA-C	76.60	142.62	108.46
1	A	1	AYA	CB-CA-C	74.48	141.68	108.46
1	D	1	AYA	CB-CA-C	74.31	141.61	108.46
1	B	1	AYA	CB-CA-C	70.34	139.84	108.46
1	B	1	AYA	CB-CA-N	17.44	136.79	110.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA
1	C	1	AYA	CA

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates 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	MMA	A	401	-	13,13,13	1.04	1 (7%)	18,18,18	4.97	2 (11%)
2	MMA	B	402	-	13,13,13	1.11	1 (7%)	18,18,18	4.96	2 (11%)
2	MMA	C	403	-	13,13,13	1.06	1 (7%)	18,18,18	4.78	2 (11%)
2	MMA	D	404	-	13,13,13	1.04	1 (7%)	18,18,18	4.92	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
2	MMA	A	401	-	-	0/4/24/24	0/1/1/1
2	MMA	B	402	-	-	0/4/24/24	0/1/1/1
2	MMA	C	403	-	-	0/4/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMA	D	404	-	-	0/4/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	MMA	O5-C1	3.11	1.49	1.41
2	D	404	MMA	O5-C1	3.08	1.49	1.41
2	C	403	MMA	O5-C1	2.92	1.49	1.41
2	A	401	MMA	O5-C1	2.77	1.48	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MMA	C7-O1-C1	20.40	144.34	113.33
2	B	402	MMA	C7-O1-C1	20.26	144.14	113.33
2	D	404	MMA	C7-O1-C1	20.09	143.87	113.33
2	C	403	MMA	C7-O1-C1	19.47	142.93	113.33
2	D	404	MMA	O5-C1-O1	5.25	123.38	110.85

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	149/149 (100%)	-0.69	1 (0%) 84 90	5, 24, 66, 93	0
1	B	149/149 (100%)	-0.64	2 (1%) 74 82	5, 21, 58, 98	0
1	C	149/149 (100%)	-0.57	1 (0%) 84 90	5, 28, 74, 100	0
1	D	149/149 (100%)	-0.57	1 (0%) 84 90	6, 31, 75, 100	0
All	All	596/596 (100%)	-0.62	5 (0%) 83 89	5, 26, 71, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	4.2
1	B	89	LEU	3.2
1	C	91	THR	3.1
1	A	89	LEU	2.2
1	B	88	ALA	2.0

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

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
1	AYA	A	1	8/9	0.25	5.11	26,26,26,26	0
1	AYA	B	1	8/9	0.19	4.01	26,26,26,26	0
1	AYA	C	1	8/9	0.19	2.38	26,26,26,26	0
1	AYA	D	1	8/9	0.20	2.21	26,26,26,26	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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
2	MMA	A	401	13/13	0.17	0.04	42,42,42,42	0
2	MMA	C	403	13/13	0.17	-0.18	44,44,44,44	0
2	MMA	D	404	13/13	0.13	-0.38	22,22,22,22	0
2	MMA	B	402	13/13	0.13	-0.41	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.