wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 05:57 PM EST

PDB ID	:	1J4T
Title	:	Structure of Artocarpin: a Lectin with Mannose Specificity (Form 2)
Authors	:	Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on	:	2001-10-30
Resolution	:	2.40 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:

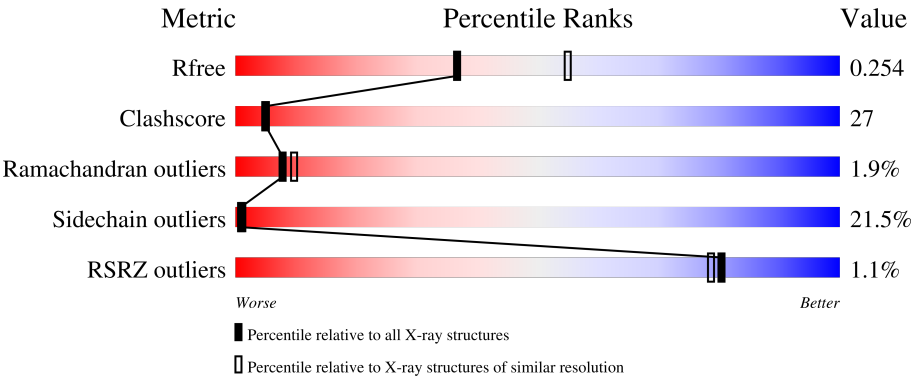
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	149	26% 46% 21% 7%
1	B	149	28% 46% 19% 7%
1	C	149	28% 46% 20% 7%
1	D	149	27% 40% 26% 7%
1	E	149	36% 39% 21% 5%

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Mol	Chain	Length	Quality of chain
1	F	149	2% 26% 44% 24% 7%
1	G	149	32% 43% 18% 7%
1	H	149	% 28% 44% 20% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	AYA	A	1	X	-	-	-
1	AYA	B	1	X	X	X	-
1	AYA	C	1	X	X	-	-
1	AYA	E	1	X	-	-	-
1	AYA	F	1	-	X	-	-
1	AYA	G	1	X	-	-	-
1	AYA	H	1	X	X	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9922 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 Artocarpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	B	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	C	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	D	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	E	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	F	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	G	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	H	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			

There are 64 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	1	AYA	ALA	modified residue	UNP Q7M1T4
E	9	SER	PRO	conflict	UNP Q7M1T4
E	20	GLU	ASP	conflict	UNP Q7M1T4
E	49	ASP	GLU	conflict	UNP Q7M1T4
E	70	LYS	ARG	conflict	UNP Q7M1T4
E	84	GLY	ALA	conflict	UNP Q7M1T4
E	145	ILE	VAL	conflict	UNP Q7M1T4
E	148	SER	ALA	conflict	UNP Q7M1T4
F	1	AYA	ALA	modified residue	UNP Q7M1T4
F	9	SER	PRO	conflict	UNP Q7M1T4
F	20	GLU	ASP	conflict	UNP Q7M1T4
F	49	ASP	GLU	conflict	UNP Q7M1T4
F	70	LYS	ARG	conflict	UNP Q7M1T4
F	84	GLY	ALA	conflict	UNP Q7M1T4
F	145	ILE	VAL	conflict	UNP Q7M1T4
F	148	SER	ALA	conflict	UNP Q7M1T4
G	1	AYA	ALA	modified residue	UNP Q7M1T4
G	9	SER	PRO	conflict	UNP Q7M1T4
G	20	GLU	ASP	conflict	UNP Q7M1T4
G	49	ASP	GLU	conflict	UNP Q7M1T4
G	70	LYS	ARG	conflict	UNP Q7M1T4
G	84	GLY	ALA	conflict	UNP Q7M1T4
G	145	ILE	VAL	conflict	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	SER	ALA	conflict	UNP Q7M1T4
H	1	AYA	ALA	modified residue	UNP Q7M1T4
H	9	SER	PRO	conflict	UNP Q7M1T4
H	20	GLU	ASP	conflict	UNP Q7M1T4
H	49	ASP	GLU	conflict	UNP Q7M1T4
H	70	LYS	ARG	conflict	UNP Q7M1T4
H	84	GLY	ALA	conflict	UNP Q7M1T4
H	145	ILE	VAL	conflict	UNP Q7M1T4
H	148	SER	ALA	conflict	UNP Q7M1T4

- Molecule 2 is water.

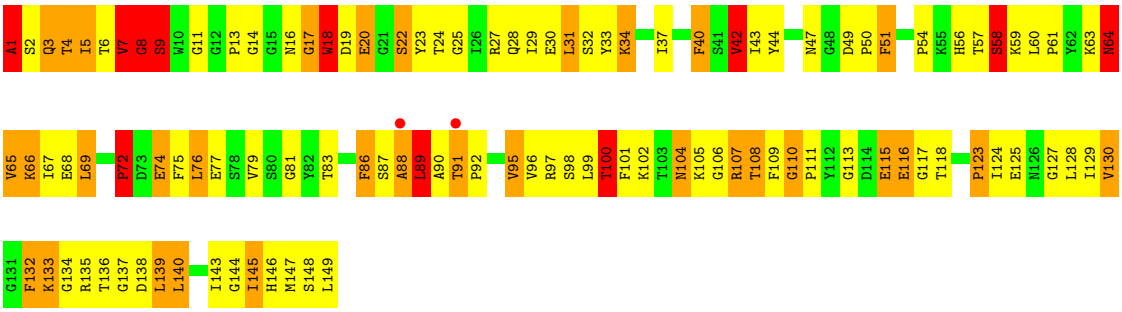
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 118 118	0	0
2	B	123	Total O 123 123	0	0
2	C	121	Total O 121 121	0	0
2	D	121	Total O 121 121	0	0
2	E	93	Total O 93 93	0	0
2	F	115	Total O 115 115	0	0
2	G	102	Total O 102 102	0	0
2	H	81	Total O 81 81	0	0

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.

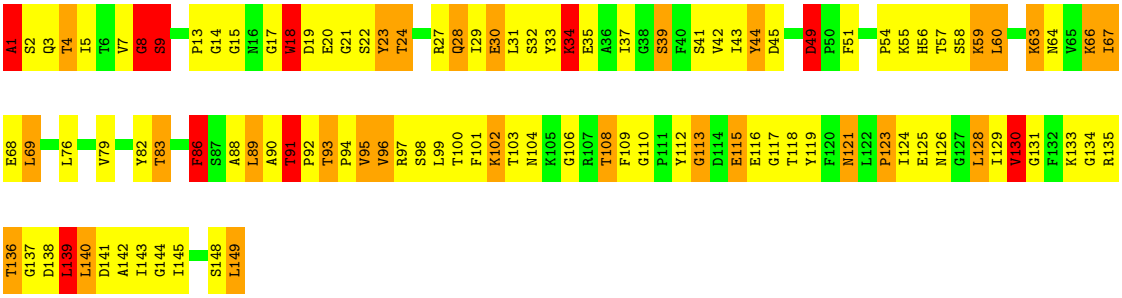
• Molecule 1: Artocarpin

Chain A:



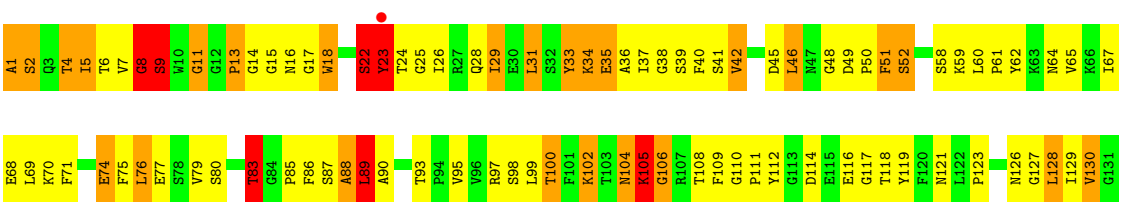
• Molecule 1: Artocarpin

Chain B:



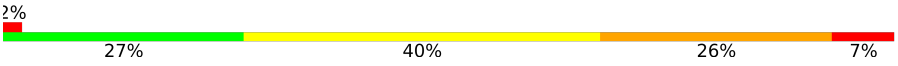
• Molecule 1: Artocarpin

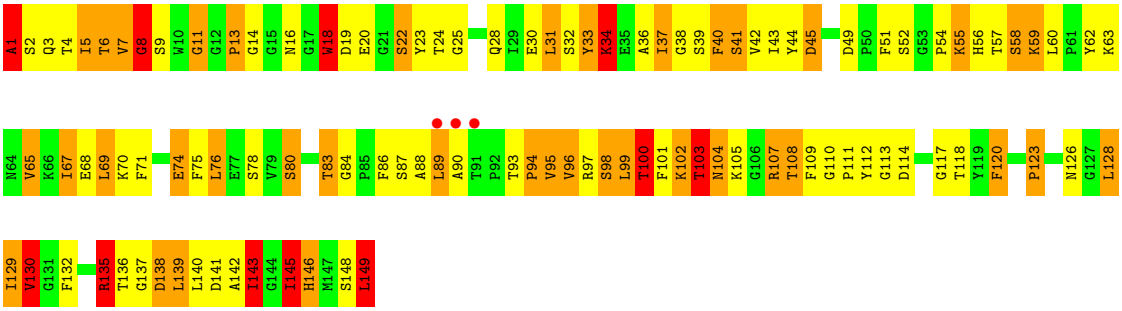
Chain C:



• Molecule 1: Artocarpin

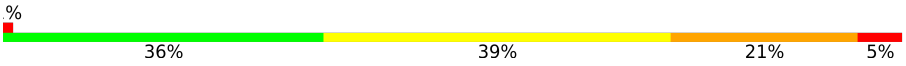
Chain D:

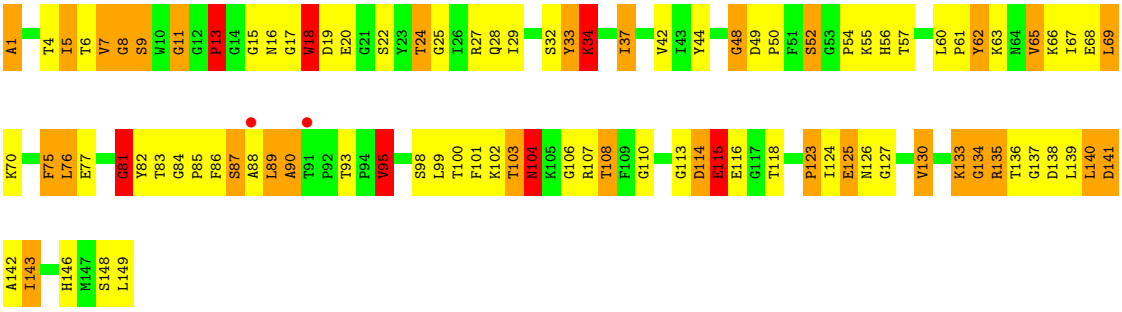




• Molecule 1: Artocarpin

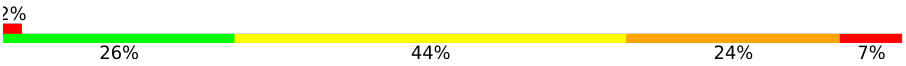
Chain E:

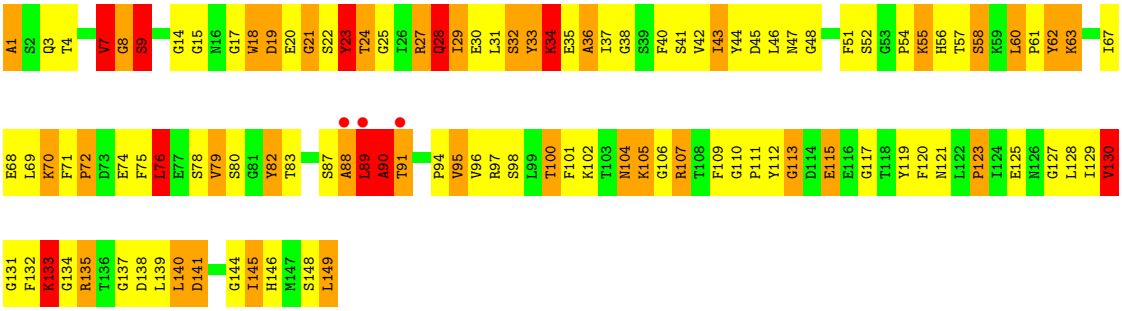




• Molecule 1: Artocarpin

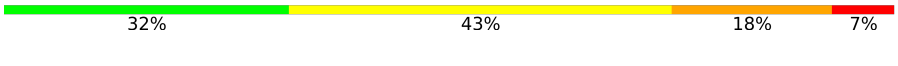
Chain F:

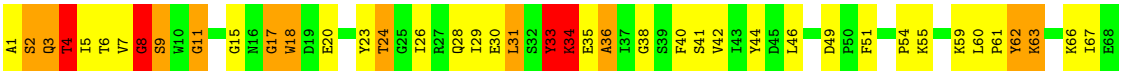


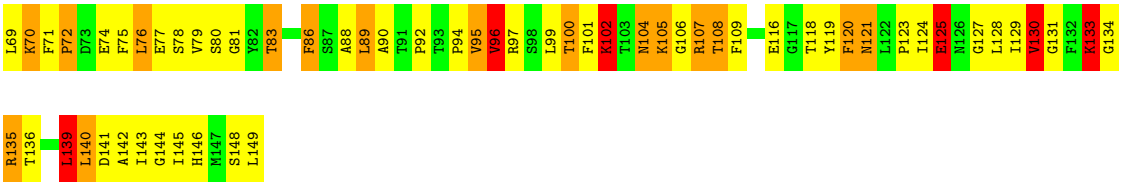


• Molecule 1: Artocarpin

Chain G:

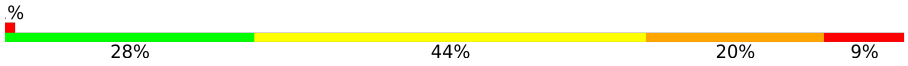


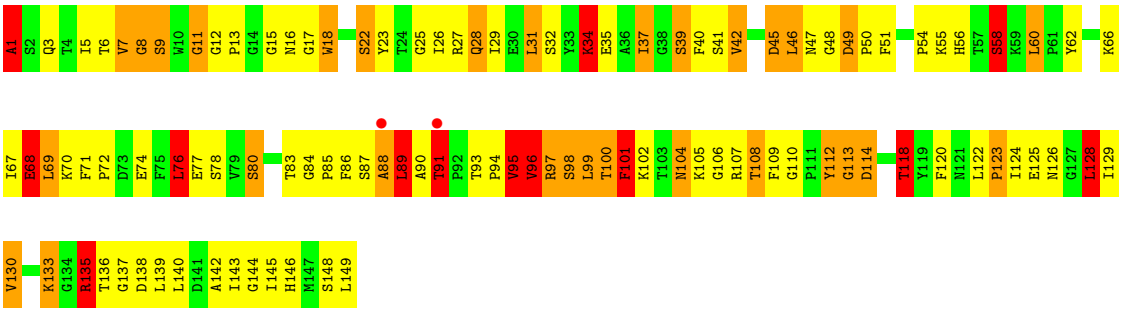




• Molecule 1: Artocarpin

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.69Å 72.19Å 92.63Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 83.5 (10.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.191 , 0.258 0.200 , 0.254	Depositor DCC
R_{free} test set	1536 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 73.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9922	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0588e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA

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	1.08	4/1155 (0.3%)	2.09	74/1569 (4.7%)
1	B	1.03	6/1155 (0.5%)	2.09	66/1569 (4.2%)
1	C	1.06	5/1155 (0.4%)	2.21	79/1569 (5.0%)
1	D	0.97	5/1155 (0.4%)	2.31	82/1569 (5.2%)
1	E	0.99	3/1151 (0.3%)	2.40	77/1565 (4.9%)
1	F	1.50	6/1151 (0.5%)	2.31	70/1565 (4.5%)
1	G	1.52	3/1155 (0.3%)	2.20	68/1569 (4.3%)
1	H	0.96	1/1155 (0.1%)	2.31	73/1569 (4.7%)
All	All	1.16	33/9232 (0.4%)	2.24	589/12544 (4.7%)

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	8
1	B	1	4
1	C	1	8
1	D	0	5
1	E	1	5
1	F	0	7
1	G	1	5
1	H	1	4
All	All	6	46

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	70	LYS	CD-CE	39.71	2.50	1.51
1	F	70	LYS	CD-CE	37.27	2.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	TYR	C-N	11.14	1.59	1.34
1	A	34	LYS	C-N	10.43	1.58	1.34
1	C	33	TYR	C-N	9.15	1.55	1.34

The worst 5 of 589 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	LYS	O-C-N	-36.39	64.47	122.70
1	G	70	LYS	CD-CE-NZ	-35.79	29.38	111.70
1	F	70	LYS	CD-CE-NZ	-35.17	30.80	111.70
1	D	34	LYS	O-C-N	-28.27	77.46	122.70
1	H	9	SER	O-C-N	-27.94	77.99	122.70

5 of 6 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
1	E	1	AYA	CA
1	G	1	AYA	CA

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	AYA	Mainchain
1	A	34	LYS	Mainchain
1	A	42	VAL	Mainchain
1	A	8	GLY	Peptide,Mainchain
1	A	9	SER	Mainchain

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	1132	0	1084	69	0
1	B	1132	0	1083	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1132	0	1084	58	0
1	D	1132	0	1080	86	0
1	E	1128	0	1071	48	0
1	F	1128	0	1067	69	0
1	G	1132	0	1081	55	0
1	H	1132	0	1082	72	0
2	A	118	0	0	7	0
2	B	123	0	0	9	0
2	C	121	0	0	4	0
2	D	121	0	0	7	0
2	E	93	0	0	4	0
2	F	115	0	0	6	0
2	G	102	0	0	6	0
2	H	81	0	0	6	0
All	All	9922	0	8632	481	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 27.

The worst 5 of 481 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:8:GLY:HA2	1:D:123:PRO:HG2	1.22	1.18
1:D:18:TRP:HZ3	1:D:136:THR:HG23	0.98	1.10
1:D:18:TRP:CZ3	1:D:136:THR:HG23	1.89	1.07
1:A:61:PRO:HD2	2:A:181:HOH:O	1.57	1.04
1:E:60:LEU:HD11	1:E:89:LEU:HD11	1.47	0.97

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	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	11 15
1	B	147/149 (99%)	136 (92%)	8 (5%)	3 (2%)	7 9
1	C	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	3 3
1	D	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	7 9
1	E	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	5 5
1	F	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	22 32
1	G	147/149 (99%)	139 (95%)	6 (4%)	2 (1%)	11 15
1	H	147/149 (99%)	128 (87%)	17 (12%)	2 (1%)	11 15
All	All	1176/1192 (99%)	1065 (91%)	89 (8%)	22 (2%)	8 10

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	110	GLY
1	B	9	SER
1	B	110	GLY
1	C	9	SER

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	120/122 (98%)	95 (79%)	25 (21%)	1 1
1	B	120/122 (98%)	93 (78%)	27 (22%)	1 1
1	C	120/122 (98%)	95 (79%)	25 (21%)	1 1
1	D	120/122 (98%)	93 (78%)	27 (22%)	1 1
1	E	119/122 (98%)	95 (80%)	24 (20%)	1 1
1	F	119/122 (98%)	95 (80%)	24 (20%)	1 1
1	G	120/122 (98%)	96 (80%)	24 (20%)	1 1
1	H	120/122 (98%)	90 (75%)	30 (25%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	958/976 (98%)	752 (78%)	206 (22%)	1 1

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	95	VAL
1	F	95	VAL
1	H	104	ASN
1	E	115	GLU
1	F	28	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	47	ASN
1	F	47	ASN
1	H	121	ASN
1	E	104	ASN
1	F	64	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)

8 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	E	1	1	6,7,8	0.81	0	5,8,10	11.28	2 (40%)
1	AYA	B	1	1	6,7,8	1.69	2 (33%)	5,8,10	11.05	5 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	AYA	H	1	1	6,7,8	1.43	1 (16%)	5,8,10	11.33	5 (100%)
1	AYA	D	1	1	6,7,8	1.80	1 (16%)	5,8,10	12.29	2 (40%)
1	AYA	G	1	1	6,7,8	2.46	1 (16%)	5,8,10	11.37	2 (40%)
1	AYA	F	1	1	6,7,8	1.63	1 (16%)	5,8,10	11.44	5 (100%)
1	AYA	A	1	1	6,7,8	1.08	0	5,8,10	11.80	4 (80%)
1	AYA	C	1	1	6,7,8	1.26	1 (16%)	5,8,10	12.06	4 (80%)

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	E	1	1	1/1/2/4	4/4/6/8	-
1	AYA	B	1	1	1/1/2/4	3/4/6/8	-
1	AYA	H	1	1	1/1/2/4	4/4/6/8	-
1	AYA	D	1	1	-	4/4/6/8	-
1	AYA	G	1	1	1/1/2/4	4/4/6/8	-
1	AYA	F	1	1	-	4/4/6/8	-
1	AYA	A	1	1	1/1/2/4	4/4/6/8	-
1	AYA	C	1	1	1/1/2/4	4/4/6/8	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	AYA	CA-N	-5.55	1.40	1.46
1	D	1	AYA	CA-N	3.60	1.50	1.46
1	F	1	AYA	CA-N	3.20	1.50	1.46
1	B	1	AYA	CA-N	-2.89	1.43	1.46
1	H	1	AYA	OT-CT	2.87	1.29	1.23

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	AYA	CB-CA-N	24.30	136.60	109.61
1	C	1	AYA	CB-CA-N	24.16	136.45	109.61
1	G	1	AYA	CB-CA-N	23.66	135.89	109.61
1	A	1	AYA	CB-CA-N	23.45	135.66	109.61
1	E	1	AYA	CB-CA-N	22.10	134.16	109.61

5 of 6 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
1	E	1	AYA	CA
1	G	1	AYA	CA

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	AYA	CB-CA-N-CT
1	A	1	AYA	OT-CT-N-CA
1	A	1	AYA	CM-CT-N-CA
1	B	1	AYA	CB-CA-N-CT
1	C	1	AYA	CB-CA-N-CT

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	AYA	1	0
1	B	1	AYA	4	0
1	H	1	AYA	2	0
1	D	1	AYA	1	0
1	F	1	AYA	2	0
1	A	1	AYA	1	0
1	C	1	AYA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	2
1	C	1
1	D	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	22:SER	C	23:TYR	N	1.20
1	D	8:GLY	C	9:SER	N	1.20
1	F	9:SER	C	10:TRP	N	1.20
1	B	89:LEU	C	90:ALA	N	1.18
1	F	90:ALA	C	91:THR	N	1.14

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, 95^{th} 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	148/149 (99%)	-0.74	2 (1%) 75 73	7, 20, 37, 60	0
1	B	148/149 (99%)	-0.62	0 100 100	11, 24, 37, 46	0
1	C	148/149 (99%)	-0.72	1 (0%) 87 86	7, 22, 34, 57	0
1	D	148/149 (99%)	-0.40	3 (2%) 65 63	11, 26, 44, 66	0
1	E	148/149 (99%)	-0.62	2 (1%) 75 73	8, 23, 47, 61	0
1	F	148/149 (99%)	-0.47	3 (2%) 65 63	9, 26, 44, 63	0
1	G	148/149 (99%)	-0.78	0 100 100	10, 21, 33, 52	0
1	H	148/149 (99%)	-0.49	2 (1%) 75 73	11, 26, 40, 60	0
All	All	1184/1192 (99%)	-0.61	13 (1%) 80 79	7, 24, 43, 66	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	91	THR	7.4
1	A	88	ALA	4.3
1	F	91	THR	4.2
1	D	91	THR	4.1
1	F	89	LEU	3.9

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. The B-factors column lists the minimum, median, 95^{th} 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
1	AYA	A	1	8/9	0.93	0.12	24,26,31,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	AYA	B	1	8/9	0.94	0.12	30,33,37,38	0
1	AYA	E	1	8/9	0.94	0.12	12,20,22,22	0
1	AYA	F	1	8/9	0.94	0.10	17,23,32,32	0
1	AYA	G	1	8/9	0.95	0.11	22,26,31,31	0
1	AYA	D	1	8/9	0.96	0.12	22,28,32,34	0
1	AYA	C	1	8/9	0.96	0.12	18,23,29,34	0
1	AYA	H	1	8/9	0.97	0.09	23,25,30,32	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.