



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:11 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 Full wwPDB X-ray Structure Validation 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/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

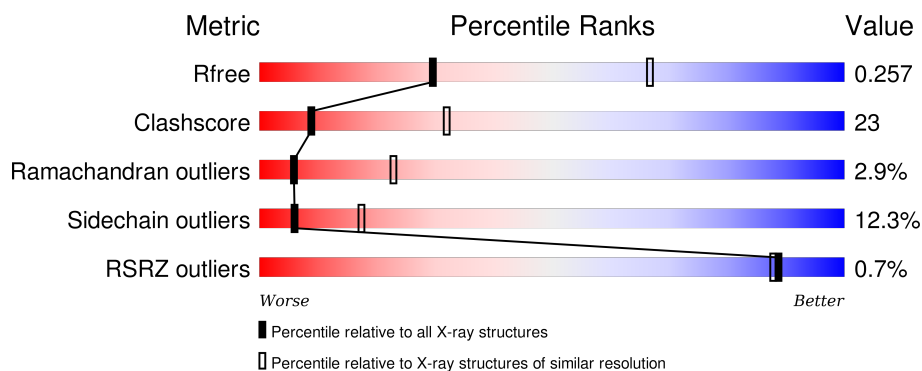
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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	149	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>45%</div> <div>11%</div> <div>•</div> </div> </div>
1	B	149	<div> <div>%</div> <div> <div></div> <div>42%</div> <div>42%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	149	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>38%</div> <div>15%</div> <div>•</div> </div> </div>
1	D	149	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>44%</div> <div>12%</div> <div>•</div> </div> </div>

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 crite-

ria:

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

2 Entry composition

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

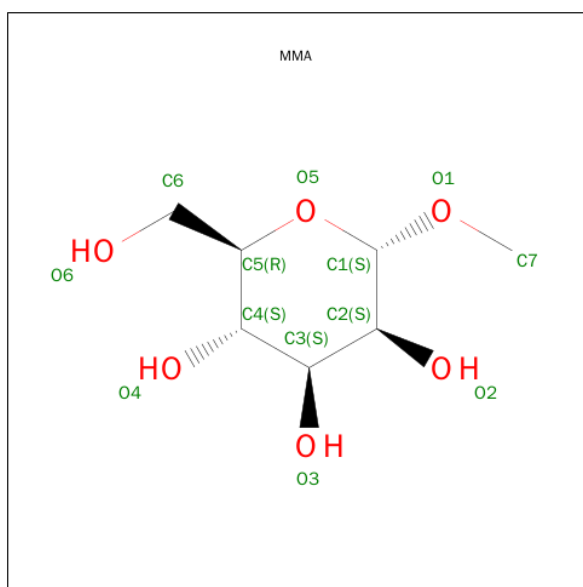
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
A	9	SER	PRO	CONFLICT	UNP Q7M1T4
A	20	GLU	ASP	CONFLICT	UNP Q7M1T4
A	49	ASP	GLU	CONFLICT	UNP Q7M1T4
A	70	LYS	ARG	CONFLICT	UNP Q7M1T4
A	84	GLY	ALA	CONFLICT	UNP Q7M1T4
A	145	ILE	VAL	CONFLICT	UNP Q7M1T4
A	148	SER	ALA	CONFLICT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

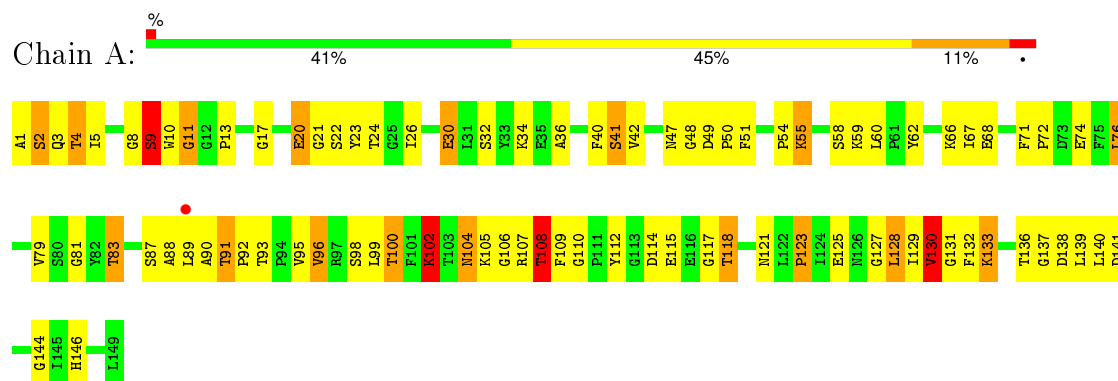
- Molecule 3 is water.

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

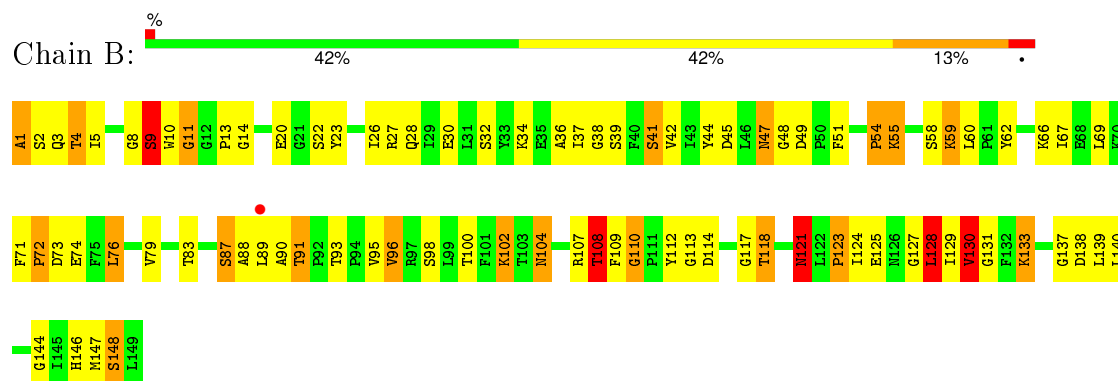
3 Residue-property plots

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.

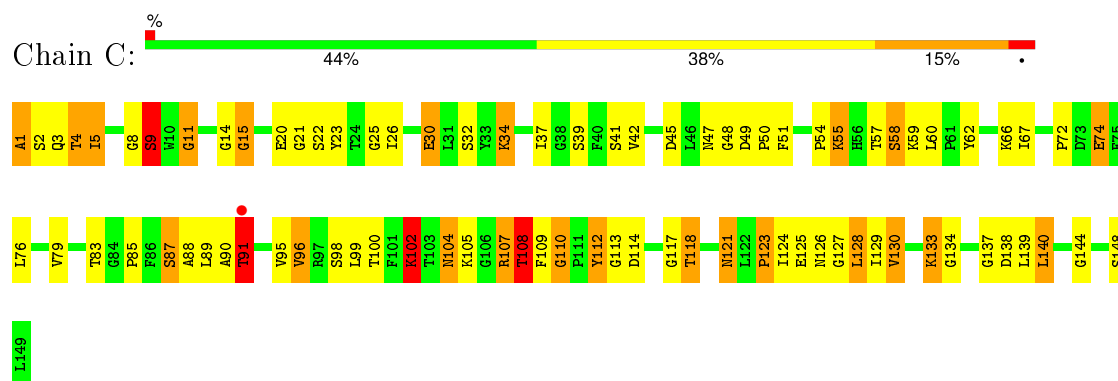
• Molecule 1: Artocarpin



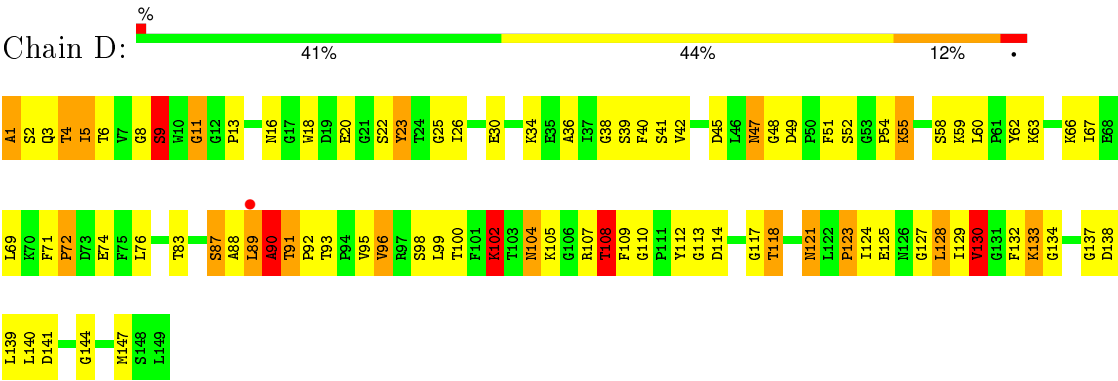
• Molecule 1: Artocarpin



• Molecule 1: Artocarpin



● Molecule 1: Artocarpin



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	129.20 Å 129.20 Å 78.61 Å 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 2.88 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.258 0.220 , 0.257	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 , 29.2	EDS
Estimated twinning fraction	0.070 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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.

All (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
1	A	2	SER	CB-CA-C	-7.53	95.79	110.10
1	B	2	SER	N-CA-CB	6.96	120.94	110.50
1	D	9	SER	N-CA-C	-6.36	93.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	SER	N-CA-C	-6.34	93.89	111.00
1	D	89	LEU	O-C-N	-6.34	112.56	122.70
1	B	9	SER	N-CA-C	-6.22	94.20	111.00
1	B	133	LYS	O-C-N	-6.22	112.62	123.20
1	A	9	SER	N-CA-C	-6.13	94.46	111.00
1	C	48	GLY	O-C-N	-5.98	113.13	122.70
1	A	117	GLY	O-C-N	-5.90	113.27	122.70
1	C	133	LYS	O-C-N	-5.89	113.19	123.20
1	A	105	LYS	O-C-N	-5.86	113.23	123.20
1	D	95	VAL	O-C-N	-5.77	113.47	122.70
1	D	92	PRO	O-C-N	-5.76	113.47	122.70
1	D	48	GLY	O-C-N	-5.76	113.49	122.70
1	B	32	SER	O-C-N	-5.76	113.49	122.70
1	C	2	SER	O-C-N	-5.75	113.50	122.70
1	C	15	GLY	O-C-N	-5.73	113.54	122.70
1	A	133	LYS	O-C-N	-5.72	113.48	123.20
1	B	45	ASP	O-C-N	-5.71	113.57	122.70
1	C	123	PRO	O-C-N	-5.69	113.59	122.70
1	A	48	GLY	O-C-N	-5.65	113.66	122.70
1	D	45	ASP	O-C-N	-5.65	113.66	122.70
1	A	131	GLY	O-C-N	-5.62	113.71	122.70
1	A	95	VAL	O-C-N	-5.59	113.76	122.70
1	C	113	GLY	O-C-N	-5.59	113.76	122.70
1	C	137	GLY	O-C-N	-5.59	113.76	122.70
1	A	127	GLY	O-C-N	-5.59	113.76	122.70
1	C	95	VAL	O-C-N	-5.57	113.79	122.70
1	C	117	GLY	O-C-N	-5.54	113.83	122.70
1	B	123	PRO	O-C-N	-5.54	113.84	122.70
1	B	95	VAL	O-C-N	-5.51	113.88	122.70
1	C	108	THR	O-C-N	-5.50	113.90	122.70
1	C	128	LEU	O-C-N	-5.50	113.90	122.70
1	A	11	GLY	O-C-N	-5.49	113.87	123.20
1	A	130	VAL	O-C-N	-5.49	113.87	123.20
1	B	76	LEU	O-C-N	-5.48	113.93	122.70
1	C	130	VAL	O-C-N	-5.48	113.88	123.20
1	B	55	LYS	O-C-N	-5.47	113.95	122.70
1	B	79	VAL	O-C-N	-5.47	113.95	122.70
1	A	41	SER	O-C-N	-5.45	113.97	122.70
1	B	36	ALA	O-C-N	-5.45	113.98	122.70
1	D	133	LYS	O-C-N	-5.45	113.94	123.20
1	B	117	GLY	O-C-N	-5.43	114.01	122.70
1	C	107	ARG	O-C-N	-5.42	114.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	GLY	O-C-N	-5.42	114.03	122.70
1	A	141	ASP	O-C-N	-5.42	114.03	122.70
1	C	144	GLY	O-C-N	-5.41	114.05	122.70
1	D	144	GLY	O-C-N	-5.39	114.07	122.70
1	D	130	VAL	O-C-N	-5.39	114.04	123.20
1	D	25	GLY	O-C-N	-5.38	114.09	122.70
1	D	123	PRO	O-C-N	-5.38	114.08	122.70
1	B	131	GLY	O-C-N	-5.38	114.09	122.70
1	D	137	GLY	O-C-N	-5.38	114.10	122.70
1	C	11	GLY	O-C-N	-5.37	114.06	123.20
1	C	51	PHE	O-C-N	-5.37	114.10	122.70
1	D	108	THR	O-C-N	-5.37	114.10	122.70
1	A	123	PRO	O-C-N	-5.36	114.12	122.70
1	C	127	GLY	O-C-N	-5.36	114.12	122.70
1	D	36	ALA	O-C-N	-5.36	114.12	122.70
1	B	146	HIS	O-C-N	-5.36	114.13	122.70
1	A	4	THR	O-C-N	-5.35	114.14	122.70
1	C	50	PRO	O-C-N	-5.34	114.15	122.70
1	C	37	ILE	O-C-N	-5.34	114.13	123.20
1	D	51	PHE	O-C-N	-5.33	114.17	122.70
1	D	134	GLY	O-C-N	-5.33	114.17	122.70
1	C	99	LEU	O-C-N	-5.33	114.18	122.70
1	D	113	GLY	O-C-N	-5.33	114.18	122.70
1	D	128	LEU	O-C-N	-5.33	114.18	122.70
1	A	79	VAL	O-C-N	-5.31	114.20	122.70
1	B	37	ILE	O-C-N	-5.31	114.17	123.20
1	D	55	LYS	O-C-N	-5.30	114.21	122.70
1	A	30	GLU	O-C-N	-5.30	114.22	122.70
1	D	90	ALA	O-C-N	-5.29	114.23	122.70
1	A	137	GLY	O-C-N	-5.28	114.25	122.70
1	D	63	LYS	O-C-N	-5.28	114.25	122.70
1	C	4	THR	O-C-N	-5.28	114.25	122.70
1	B	108	THR	O-C-N	-5.27	114.26	122.70
1	B	27	ARG	O-C-N	-5.27	114.27	122.70
1	C	102	LYS	O-C-N	-5.27	114.27	122.70
1	D	38	GLY	O-C-N	-5.25	114.30	122.70
1	C	55	LYS	O-C-N	-5.25	114.31	122.70
1	A	51	PHE	O-C-N	-5.24	114.31	122.70
1	B	69	LEU	O-C-N	-5.24	114.31	122.70
1	D	117	GLY	O-C-N	-5.24	114.32	122.70
1	A	102	LYS	O-C-N	-5.23	114.33	122.70
1	D	4	THR	O-C-N	-5.23	114.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	18	TRP	O-C-N	-5.23	114.33	122.70
1	A	128	LEU	O-C-N	-5.23	114.34	122.70
1	A	108	THR	O-C-N	-5.22	114.35	122.70
1	B	39	SER	O-C-N	-5.22	114.35	122.70
1	A	10	TRP	O-C-N	-5.22	114.33	123.20
1	C	79	VAL	O-C-N	-5.21	114.36	122.70
1	A	55	LYS	O-C-N	-5.19	114.40	122.70
1	A	99	LEU	O-C-N	-5.19	114.40	122.70
1	A	24	THR	O-C-N	-5.19	114.38	123.20
1	A	17	GLY	O-C-N	-5.19	114.40	122.70
1	B	130	VAL	O-C-N	-5.18	114.39	123.20
1	D	69	LEU	O-C-N	-5.18	114.41	122.70
1	B	148	SER	O-C-N	-5.18	114.41	122.70
1	C	126	ASN	O-C-N	-5.18	114.39	123.20
1	A	40	PHE	O-C-N	-5.18	114.42	122.70
1	A	50	PRO	O-C-N	-5.17	114.43	122.70
1	D	3	GLN	O-C-N	-5.17	114.43	122.70
1	C	91	THR	N-CA-C	-5.17	97.05	111.00
1	C	14	GLY	O-C-N	-5.17	114.42	123.20
1	C	45	ASP	O-C-N	-5.17	114.43	122.70
1	D	11	GLY	O-C-N	-5.17	114.42	123.20
1	B	137	GLY	O-C-N	-5.16	114.45	122.70
1	D	5	ILE	O-C-N	-5.16	114.45	122.70
1	B	4	THR	O-C-N	-5.15	114.45	122.70
1	B	121	ASN	O-C-N	-5.15	114.46	122.70
1	B	10	TRP	O-C-N	-5.15	114.45	123.20
1	C	58	SER	O-C-N	-5.15	114.47	122.70
1	A	21	GLY	O-C-N	-5.14	114.47	122.70
1	B	11	GLY	O-C-N	-5.14	114.46	123.20
1	A	136	THR	O-C-N	-5.14	114.47	123.20
1	D	127	GLY	O-C-N	-5.14	114.48	122.70
1	A	144	GLY	O-C-N	-5.13	114.48	122.70
1	C	5	ILE	O-C-N	-5.13	114.49	122.70
1	D	40	PHE	O-C-N	-5.13	114.49	122.70
1	A	106	GLY	O-C-N	-5.12	114.52	122.70
1	C	85	PRO	O-C-N	-5.12	114.52	122.70
1	C	105	LYS	O-C-N	-5.12	114.50	123.20
1	D	47	ASN	O-C-N	-5.11	114.51	123.20
1	B	51	PHE	O-C-N	-5.11	114.53	122.70
1	C	32	SER	O-C-N	-5.10	114.54	122.70
1	A	129	ILE	O-C-N	-5.10	114.55	122.70
1	B	54	PRO	O-C-N	-5.09	114.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	GLN	O-C-N	-5.09	114.56	122.70
1	C	112	TYR	O-C-N	-5.09	114.55	123.20
1	A	83	THR	O-C-N	-5.09	114.55	123.20
1	D	6	THR	O-C-N	-5.08	114.57	122.70
1	D	102	LYS	O-C-N	-5.08	114.57	122.70
1	A	3	GLN	O-C-N	-5.08	114.57	122.70
1	C	30	GLU	O-C-N	-5.08	114.57	122.70
1	B	28	GLN	O-C-N	-5.08	114.58	122.70
1	B	144	GLY	O-C-N	-5.07	114.58	122.70
1	C	25	GLY	O-C-N	-5.07	114.58	122.70
1	D	52	SER	O-C-N	-5.07	114.58	123.20
1	B	3	GLN	O-C-N	-5.07	114.59	122.70
1	B	14	GLY	O-C-N	-5.07	114.59	123.20
1	B	59	LYS	O-C-N	-5.07	114.59	122.70
1	A	32	SER	O-C-N	-5.06	114.60	122.70
1	B	41	SER	O-C-N	-5.06	114.60	122.70
1	C	134	GLY	O-C-N	-5.06	114.60	122.70
1	B	47	ASN	O-C-N	-5.06	114.60	123.20
1	B	38	GLY	O-C-N	-5.05	114.61	122.70
1	D	39	SER	O-C-N	-5.05	114.62	122.70
1	B	73	ASP	O-C-N	-5.05	114.62	122.70
1	D	99	LEU	O-C-N	-5.05	114.63	122.70
1	A	20	GLU	O-C-N	-5.04	114.63	123.20
1	A	76	LEU	O-C-N	-5.03	114.65	122.70
1	C	74	GLU	O-C-N	-5.03	114.65	122.70
1	D	105	LYS	O-C-N	-5.03	114.65	123.20
1	A	115	GLU	O-C-N	-5.03	114.66	122.70
1	C	124	ILE	O-C-N	-5.03	114.66	122.70
1	B	113	GLY	O-C-N	-5.02	114.66	122.70
1	B	127	GLY	O-C-N	-5.02	114.66	122.70
1	D	141	ASP	O-C-N	-5.02	114.67	122.70
1	A	146	HIS	O-C-N	-5.02	114.67	122.70
1	C	21	GLY	O-C-N	-5.02	114.67	122.70
1	D	23	TYR	O-C-N	-5.02	114.67	122.70
1	A	36	ALA	O-C-N	-5.01	114.69	122.70
1	B	128	LEU	O-C-N	-5.01	114.69	122.70
1	C	140	LEU	O-C-N	-5.00	114.69	122.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA

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Mol	Chain	Res	Type	Atom
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 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	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

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 23.

All (210) 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: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
1:A:22:SER:H	1:C:47:ASN:HD21	1.34	0.76
1:C:96:VAL:HG13	1:C:140:LEU:O	1.86	0.76
1:A:66:LYS:CD	3:A:268:HOH:O	2.33	0.76
1:D:74:GLU:OE2	1:D:107:ARG:HD3	1.86	0.75
1:D:20:GLU:HG2	1:D:54:PRO:HD2	1.69	0.74
1:B:96:VAL:HG13	1:B:140:LEU:O	1.87	0.73
1:B:47:ASN:HD21	1:D:22:SER:H	1.37	0.73
1:B:8:GLY:O	1:B:9:SER:HB2	1.88	0.72
1:C:8:GLY:O	1:C:9:SER:HB2	1.89	0.72
1:C:74:GLU:OE2	1:C:107:ARG:HD3	1.90	0.72
1:B:74:GLU:OE2	1:B:107:ARG:HD3	1.90	0.71
1:A:68:GLU:OE2	3:A:282:HOH:O	2.08	0.71
1:B:74:GLU:HA	1:B:104:ASN:HD21	1.56	0.71
1:A:74:GLU:OE2	1:A:107:ARG:HD3	1.91	0.71
1:A:66:LYS:HD2	3:A:268:HOH:O	1.89	0.71
1:A:8:GLY:O	1:A:9:SER:HB2	1.90	0.71
1:B:20:GLU:HG2	1:B:54:PRO:HD2	1.73	0.71
1:A:59:LYS:HD2	3:A:288:HOH:O	1.90	0.70
1:A:30:GLU:HG2	1:A:66:LYS:HG2	1.72	0.69
1:B:109:PHE:O	3:B:306:HOH:O	2.10	0.69
1:D:8:GLY:O	1:D:9:SER:HB2	1.91	0.69
1:C:20:GLU:HG2	1:C:54:PRO:HD2	1.74	0.68
1:C:104:ASN:HD22	1:C:104:ASN:N	1.91	0.68
1:D:104:ASN:N	1:D:104:ASN:HD22	1.92	0.67
1:B:22:SER:H	1:D:47:ASN:HD21	1.42	0.67
1:A:68:GLU:HB3	3:A:285:HOH:O	1.95	0.67
1:A:47:ASN:HD21	1:C:22:SER:H	1.43	0.67
1:A:96:VAL:HG13	1:A:140:LEU:O	1.94	0.67
1:A:104:ASN:HD22	1:A:104:ASN:N	1.93	0.66
1:D:89:LEU:CD1	1:D:139:LEU:HD21	2.26	0.66
1:A:66:LYS:CB	3:A:268:HOH:O	2.43	0.65
1:D:96:VAL:HG13	1:D:140:LEU:O	1.95	0.65
1:D:23:TYR:O	1:D:130:VAL:HG22	1.96	0.65
1:C:60:LEU:H	1:C:60:LEU:HD22	1.62	0.64
1:C:74:GLU:HA	1:C:104:ASN:HD21	1.62	0.64
1:A:81:GLY:HA2	3:A:283:HOH:O	1.96	0.64
1:C:8:GLY:HA2	1:D:123:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:N	1:B:104:ASN:HD22	1.95	0.63
1:C:102:LYS:HD2	1:C:108:THR:HB	1.81	0.63
1:B:89:LEU:CD1	1:B:139:LEU:HD21	2.28	0.62
1:C:89:LEU:CD1	1:C:139:LEU:HD21	2.29	0.62
1:D:67:ILE:HG23	1:D:109:PHE:CE2	2.34	0.62
1:A:60:LEU:H	1:A:60:LEU:HD22	1.65	0.62
1:A:20:GLU:HG2	1:A:54:PRO:HD2	1.81	0.62
1:A:89:LEU:CD1	1:A:139:LEU:HD21	2.30	0.61
1:D:60:LEU:HD22	1:D:60:LEU:H	1.64	0.61
1:D:74:GLU:HA	1:D:104:ASN:HD21	1.64	0.61
1:D:30:GLU:HG2	1:D:66:LYS:HG2	1.82	0.61
1:A:74:GLU:HA	1:A:104:ASN:HD21	1.66	0.61
1:A:67:ILE:HG23	1:A:109:PHE:CE2	2.36	0.61
1:C:23:TYR:O	1:C:130:VAL:HG22	2.00	0.60
1:A:102:LYS:HD2	1:A:108:THR:HB	1.83	0.60
1:C:30:GLU:HG2	1:C:66:LYS:HG2	1.83	0.60
1:B:30:GLU:HG2	1:B:66:LYS:HG2	1.84	0.60
1:A:23:TYR:O	1:A:130:VAL:HG22	2.02	0.59
1:B:23:TYR:O	1:B:130:VAL:HG22	2.02	0.59
1:B:8:GLY:O	1:B:9:SER:CB	2.49	0.59
1:C:125:GLU:CD	1:D:133:LYS:HE2	2.23	0.59
1:A:133:LYS:HE2	1:B:125:GLU:OE1	2.03	0.59
1:D:4:THR:HG22	3:D:257:HOH:O	2.03	0.58
1:D:89:LEU:HD12	1:D:139:LEU:HD21	1.85	0.58
1:C:125:GLU:OE1	1:D:133:LYS:HE2	2.03	0.58
1:B:128:LEU:HG	1:D:1:AYA:HM2	1.84	0.58
1:B:58:SER:HB2	1:B:138:ASP:O	2.04	0.57
1:A:8:GLY:O	1:A:9:SER:CB	2.52	0.57
1:D:23:TYR:O	1:D:130:VAL:CG2	2.52	0.57
1:B:89:LEU:HD12	1:B:139:LEU:HD21	1.85	0.57
1:A:58:SER:HB2	1:A:138:ASP:O	2.04	0.57
1:C:83:THR:CG2	1:C:118:THR:HG23	2.34	0.57
1:C:67:ILE:HG23	1:C:109:PHE:CE2	2.40	0.57
1:B:102:LYS:HG3	1:B:108:THR:HB	1.86	0.57
1:C:8:GLY:O	1:C:9:SER:CB	2.52	0.56
1:C:125:GLU:OE2	1:D:133:LYS:HE2	2.04	0.56
1:D:102:LYS:HD2	1:D:108:THR:HB	1.88	0.56
1:C:89:LEU:HD12	1:C:139:LEU:HD21	1.87	0.56
1:D:8:GLY:O	1:D:9:SER:CB	2.53	0.56
1:C:60:LEU:H	1:C:60:LEU:CD2	2.19	0.56
1:C:123:PRO:HD2	1:D:8:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LYS:HE2	1:D:125:GLU:OE2	2.07	0.55
1:A:89:LEU:HD12	1:A:139:LEU:HD21	1.89	0.55
1:A:60:LEU:HD21	1:A:138:ASP:HB3	1.88	0.54
1:A:71:PHE:CE2	1:C:1:AYA:OT	2.61	0.54
1:D:60:LEU:CD2	1:D:60:LEU:H	2.20	0.54
1:A:60:LEU:H	1:A:60:LEU:CD2	2.21	0.54
1:A:133:LYS:HE2	1:B:125:GLU:CD	2.28	0.54
1:D:83:THR:CG2	1:D:118:THR:HG23	2.37	0.54
1:B:67:ILE:HG23	1:B:109:PHE:CE2	2.43	0.53
1:C:23:TYR:O	1:C:130:VAL:CG2	2.57	0.53
1:B:60:LEU:H	1:B:60:LEU:HD22	1.73	0.53
1:C:39:SER:HB3	1:C:57:THR:HA	1.91	0.53
1:B:83:THR:CG2	1:B:118:THR:HG23	2.39	0.53
1:C:60:LEU:HD21	1:C:138:ASP:HB3	1.91	0.52
1:A:125:GLU:OE1	1:B:133:LYS:HE2	2.09	0.52
1:A:83:THR:CG2	1:A:118:THR:HG23	2.40	0.52
1:D:89:LEU:HD13	1:D:139:LEU:HD21	1.91	0.52
1:C:58:SER:HB2	1:C:138:ASP:O	2.10	0.51
1:C:60:LEU:HB3	1:C:62:TYR:CE1	2.46	0.51
1:D:58:SER:HB2	1:D:138:ASP:O	2.12	0.50
1:A:4:THR:O	1:A:5:ILE:C	2.48	0.50
1:B:71:PHE:CE1	1:B:72:PRO:HB3	2.47	0.50
1:B:60:LEU:HD21	1:B:138:ASP:HB3	1.94	0.50
1:D:13:PRO:HD2	1:D:93:THR:OG1	2.11	0.49
1:A:60:LEU:HB3	1:A:62:TYR:CE1	2.47	0.49
1:B:89:LEU:O	1:B:91:THR:CG2	2.51	0.49
1:B:96:VAL:CG2	1:B:96:VAL:O	2.59	0.49
1:B:87:SER:O	1:B:88:ALA:C	2.50	0.49
1:C:41:SER:HB3	1:C:55:LYS:HA	1.93	0.49
1:C:26:ILE:HD11	1:C:129:ILE:HG22	1.94	0.49
1:C:89:LEU:HD13	1:C:139:LEU:HD21	1.94	0.49
1:A:125:GLU:CD	1:B:133:LYS:HE2	2.33	0.49
1:D:89:LEU:O	1:D:90:ALA:C	2.51	0.48
1:B:89:LEU:HD13	1:B:139:LEU:HD21	1.95	0.48
1:B:23:TYR:O	1:B:130:VAL:CG2	2.60	0.48
1:B:60:LEU:H	1:B:60:LEU:CD2	2.25	0.48
1:C:87:SER:O	1:C:88:ALA:C	2.49	0.48
1:D:71:PHE:CE1	1:D:72:PRO:HB3	2.47	0.48
1:D:60:LEU:HD21	1:D:138:ASP:HB3	1.94	0.48
1:A:66:LYS:HB3	3:A:268:HOH:O	2.09	0.48
1:A:23:TYR:O	1:A:130:VAL:CG2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:O	1:B:60:LEU:C	2.52	0.48
1:A:22:SER:H	1:C:47:ASN:ND2	2.06	0.48
1:D:60:LEU:HB3	1:D:62:TYR:CE1	2.49	0.48
1:D:11:GLY:HA2	1:D:83:THR:OG1	2.13	0.48
1:A:89:LEU:HD13	1:A:139:LEU:HD21	1.94	0.47
1:B:109:PHE:HB2	3:B:306:HOH:O	2.14	0.47
1:D:60:LEU:HD22	1:D:60:LEU:N	2.28	0.47
1:A:133:LYS:HE2	1:B:125:GLU:OE2	2.15	0.47
1:D:104:ASN:N	1:D:104:ASN:ND2	2.62	0.47
1:C:59:LYS:O	1:C:60:LEU:C	2.50	0.47
1:A:11:GLY:HA2	1:A:83:THR:OG1	2.15	0.47
1:C:4:THR:O	1:C:5:ILE:C	2.52	0.47
1:B:11:GLY:HA2	1:B:83:THR:OG1	2.14	0.47
1:D:41:SER:HB3	1:D:55:LYS:HA	1.97	0.47
1:A:13:PRO:HD2	1:A:93:THR:OG1	2.14	0.47
1:D:67:ILE:HG23	1:D:109:PHE:CD2	2.49	0.46
1:D:59:LYS:O	1:D:60:LEU:C	2.53	0.46
1:B:4:THR:O	1:B:5:ILE:C	2.50	0.46
1:B:41:SER:HB3	1:B:55:LYS:HA	1.97	0.46
1:B:124:ILE:CD1	1:B:147:MET:HE3	2.46	0.46
1:B:22:SER:H	1:D:47:ASN:ND2	2.11	0.46
1:A:26:ILE:HD13	1:A:132:PHE:HE1	1.80	0.46
1:A:87:SER:O	1:A:88:ALA:C	2.54	0.46
1:A:125:GLU:OE2	1:B:133:LYS:HE2	2.14	0.46
1:D:26:ILE:HD11	1:D:129:ILE:HG22	1.97	0.46
1:A:8:GLY:HA2	1:B:123:PRO:HD2	1.97	0.46
1:C:60:LEU:N	1:C:60:LEU:HD22	2.27	0.46
1:C:148:SER:HA	1:D:5:ILE:HD11	1.98	0.46
1:B:26:ILE:HD11	1:B:129:ILE:HG22	1.96	0.46
1:A:100:THR:CG2	3:A:283:HOH:O	2.63	0.46
1:C:11:GLY:HA2	1:C:83:THR:OG1	2.16	0.46
1:B:60:LEU:HB3	1:B:62:TYR:CE1	2.52	0.45
1:A:67:ILE:HG23	1:A:109:PHE:CD2	2.51	0.45
1:B:60:LEU:N	1:B:60:LEU:HD22	2.32	0.45
1:C:98:SER:HB2	1:C:114:ASP:O	2.17	0.45
1:A:59:LYS:O	1:A:60:LEU:C	2.53	0.45
1:D:4:THR:O	1:D:5:ILE:C	2.52	0.45
1:A:98:SER:HB2	1:A:114:ASP:O	2.17	0.45
1:D:20:GLU:CG	1:D:54:PRO:HD2	2.44	0.45
1:B:121:ASN:O	1:B:123:PRO:HD3	2.17	0.45
1:C:4:THR:HG21	1:C:22:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASN:O	1:D:123:PRO:HD3	2.17	0.44
1:C:83:THR:HG22	1:C:118:THR:HG23	1.99	0.44
1:C:104:ASN:H	1:C:104:ASN:HD22	1.66	0.44
1:D:83:THR:HG22	1:D:118:THR:HG23	1.99	0.44
1:C:20:GLU:CG	1:C:54:PRO:HD2	2.47	0.44
1:A:123:PRO:HD2	1:B:8:GLY:HA2	1.98	0.44
1:A:123:PRO:HB2	1:B:8:GLY:HA2	1.99	0.44
1:C:67:ILE:HG23	1:C:109:PHE:CD2	2.53	0.44
1:A:41:SER:HB3	1:A:55:LYS:HA	1.98	0.44
1:A:60:LEU:N	1:A:60:LEU:HD22	2.32	0.44
1:A:47:ASN:ND2	1:C:22:SER:H	2.12	0.44
1:C:39:SER:CB	1:C:57:THR:HA	2.48	0.44
1:A:98:SER:HA	1:A:112:TYR:O	2.18	0.44
1:C:133:LYS:HE2	1:D:125:GLU:CD	2.38	0.43
1:B:96:VAL:HG22	1:B:96:VAL:O	2.18	0.43
1:B:109:PHE:O	1:B:110:GLY:O	2.35	0.43
1:A:66:LYS:HB2	3:A:268:HOH:O	2.11	0.43
1:D:98:SER:HB2	1:D:114:ASP:O	2.17	0.43
1:B:104:ASN:H	1:B:104:ASN:HD22	1.66	0.43
1:D:98:SER:HA	1:D:112:TYR:O	2.19	0.43
1:B:98:SER:HA	1:B:112:TYR:O	2.19	0.43
1:A:5:ILE:HD11	1:B:148:SER:HA	2.00	0.43
1:C:121:ASN:O	1:C:123:PRO:HD3	2.18	0.43
1:C:89:LEU:O	1:C:91:THR:CG2	2.48	0.42
1:B:109:PHE:O	1:B:110:GLY:C	2.58	0.42
1:A:104:ASN:ND2	1:A:104:ASN:N	2.63	0.42
1:B:20:GLU:OE2	1:B:44:TYR:OH	2.24	0.42
1:A:4:THR:HG22	3:A:310:HOH:O	2.17	0.42
1:D:26:ILE:HD13	1:D:132:PHE:HE1	1.84	0.42
1:C:104:ASN:N	1:C:104:ASN:ND2	2.62	0.42
1:B:13:PRO:HD2	1:B:93:THR:OG1	2.19	0.42
1:D:87:SER:O	1:D:88:ALA:C	2.58	0.42
1:B:20:GLU:CG	1:B:54:PRO:HD2	2.46	0.42
1:B:83:THR:HG22	1:B:118:THR:HG23	2.01	0.41
1:C:83:THR:HG23	1:C:118:THR:HG23	2.00	0.41
1:C:98:SER:HA	1:C:112:TYR:O	2.20	0.41
1:D:124:ILE:CD1	1:D:147:MET:HE3	2.50	0.41
1:D:104:ASN:H	1:D:104:ASN:HD22	1.68	0.41
1:B:47:ASN:ND2	1:D:22:SER:H	2.11	0.41
1:C:109:PHE:O	1:C:110:GLY:O	2.38	0.41
1:B:98:SER:HB2	1:B:114:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HG23	1:B:109:PHE:CD2	2.56	0.40
1:A:104:ASN:H	1:A:104:ASN:HD22	1.68	0.40
1:A:66:LYS:HD3	3:A:268:HOH:O	2.11	0.40
1:B:1:AYA:OT	1:D:71:PHE:CE2	2.75	0.40

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	Interatomic distance (Å)	Clash overlap (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%)	6	25
1	B	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	6	25
1	C	147/149 (99%)	133 (90%)	9 (6%)	5 (3%)	5	19
1	D	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	6	25
All	All	588/596 (99%)	528 (90%)	43 (7%)	17 (3%)	6	23

All (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
1	B	110	GLY

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Mol	Chain	Res	Type
1	C	9	SER
1	C	90	ALA
1	C	110	GLY
1	D	9	SER
1	D	110	GLY
1	B	34	LYS
1	A	34	LYS
1	C	34	LYS
1	D	34	LYS
1	D	90	ALA
1	C	15	GLY

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%)	7	19
1	B	120/122 (98%)	105 (88%)	15 (12%)	6	17
1	C	120/122 (98%)	105 (88%)	15 (12%)	6	17
1	D	120/122 (98%)	105 (88%)	15 (12%)	6	17
All	All	480/488 (98%)	421 (88%)	59 (12%)	6	17

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	49	ASP
1	A	72	PRO
1	A	76	LEU
1	A	91	THR
1	A	96	VAL
1	A	100	THR
1	A	102	LYS
1	A	104	ASN
1	A	108	THR

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Mol	Chain	Res	Type
1	A	118	THR
1	A	121	ASN
1	A	128	LEU
1	A	130	VAL
1	B	42	VAL
1	B	49	ASP
1	B	72	PRO
1	B	76	LEU
1	B	87	SER
1	B	91	THR
1	B	96	VAL
1	B	100	THR
1	B	102	LYS
1	B	104	ASN
1	B	108	THR
1	B	118	THR
1	B	121	ASN
1	B	128	LEU
1	B	130	VAL
1	C	34	LYS
1	C	42	VAL
1	C	49	ASP
1	C	72	PRO
1	C	76	LEU
1	C	87	SER
1	C	91	THR
1	C	96	VAL
1	C	100	THR
1	C	102	LYS
1	C	104	ASN
1	C	108	THR
1	C	118	THR
1	C	121	ASN
1	C	128	LEU
1	D	42	VAL
1	D	49	ASP
1	D	72	PRO
1	D	76	LEU
1	D	87	SER
1	D	91	THR
1	D	96	VAL
1	D	100	THR

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Mol	Chain	Res	Type
1	D	102	LYS
1	D	104	ASN
1	D	108	THR
1	D	118	THR
1	D	121	ASN
1	D	128	LEU
1	D	130	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules 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	6,7,8	1.40	1 (16%)	7,8,10	11.45	4 (57%)
1	AYA	B	1	1	6,7,8	1.10	0	7,8,10	11.49	4 (57%)
1	AYA	C	1	1	6,7,8	0.77	0	7,8,10	11.52	4 (57%)
1	AYA	D	1	1	6,7,8	1.15	1 (16%)	7,8,10	10.58	4 (57%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	AYA	CA-N	2.19	1.48	1.46
1	A	1	AYA	CA-N	3.31	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	AYA	C-CA-N	-14.27	80.66	110.64
1	D	1	AYA	C-CA-N	-13.40	82.47	110.64
1	B	1	AYA	C-CA-N	-12.98	83.36	110.64
1	A	1	AYA	C-CA-N	-12.84	83.65	110.64
1	D	1	AYA	O-C-CA	-10.95	91.34	124.64
1	B	1	AYA	O-C-CA	-10.89	91.53	124.64
1	A	1	AYA	O-C-CA	-10.59	92.42	124.64
1	C	1	AYA	O-C-CA	-10.51	92.67	124.64
1	D	1	AYA	CA-N-CT	8.75	135.02	121.46
1	B	1	AYA	CA-N-CT	9.59	136.32	121.46
1	C	1	AYA	CA-N-CT	10.77	138.14	121.46
1	A	1	AYA	CA-N-CT	13.19	141.90	121.46
1	D	1	AYA	CB-CA-N	20.06	132.96	109.61
1	A	1	AYA	CB-CA-N	21.48	134.62	109.61
1	C	1	AYA	CB-CA-N	22.23	135.50	109.61
1	B	1	AYA	CB-CA-N	23.34	136.79	109.61

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	AYA	1	0
1	C	1	AYA	1	0
1	D	1	AYA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	4.65	2 (11%)
2	MMA	B	402	-	13,13,13	1.11	1 (7%)	18,18,18	4.63	2 (11%)
2	MMA	C	403	-	13,13,13	1.06	1 (7%)	18,18,18	4.47	2 (11%)
2	MMA	D	404	-	13,13,13	1.03	1 (7%)	18,18,18	4.60	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
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	A	401	MMA	O5-C1	2.77	1.48	1.41
2	C	403	MMA	O5-C1	2.92	1.49	1.41
2	D	404	MMA	O5-C1	3.08	1.49	1.41
2	B	402	MMA	O5-C1	3.11	1.49	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MMA	O5-C1-O1	4.69	122.15	110.88
2	B	402	MMA	O5-C1-O1	5.07	123.08	110.88
2	C	403	MMA	O5-C1-O1	5.09	123.12	110.88
2	D	404	MMA	O5-C1-O1	5.20	123.38	110.88
2	C	403	MMA	C7-O1-C1	18.11	142.93	113.29
2	D	404	MMA	C7-O1-C1	18.68	143.87	113.29
2	B	402	MMA	C7-O1-C1	18.85	144.14	113.29
2	A	401	MMA	C7-O1-C1	18.97	144.34	113.29

There are no chirality outliers.

There are no torsion outliers.

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

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	148/149 (99%)	-0.73	1 (0%) 89 88	5, 24, 66, 93	0
1	B	148/149 (99%)	-0.68	1 (0%) 89 88	5, 21, 58, 98	0
1	C	148/149 (99%)	-0.62	1 (0%) 89 88	5, 29, 74, 100	0
1	D	148/149 (99%)	-0.62	1 (0%) 89 88	6, 31, 75, 100	0
All	All	592/596 (99%)	-0.66	4 (0%) 89 88	5, 26, 71, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	3.9
1	B	89	LEU	3.0
1	C	91	THR	2.9
1	A	89	LEU	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	AYA	A	1	8/9	0.95	0.25	-	26,26,26,26	0
1	AYA	B	1	8/9	0.95	0.19	-	26,26,26,26	0
1	AYA	C	1	8/9	0.95	0.19	-	26,26,26,26	0
1	AYA	D	1	8/9	0.96	0.20	-	26,26,26,26	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MMA	A	401	13/13	0.96	0.17	0.04	42,42,42,42	0
2	MMA	C	403	13/13	0.96	0.17	-0.17	44,44,44,44	0
2	MMA	D	404	13/13	0.96	0.13	-0.39	22,22,22,22	0
2	MMA	B	402	13/13	0.97	0.13	-0.41	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.