Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:11 PM GMT

PDB ID	:	1J4S
Title	:	Structure of Artocarpin: a Lectin with Mannose Specificity (Form 1)
Authors	:	Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on	:	2001-10-30
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

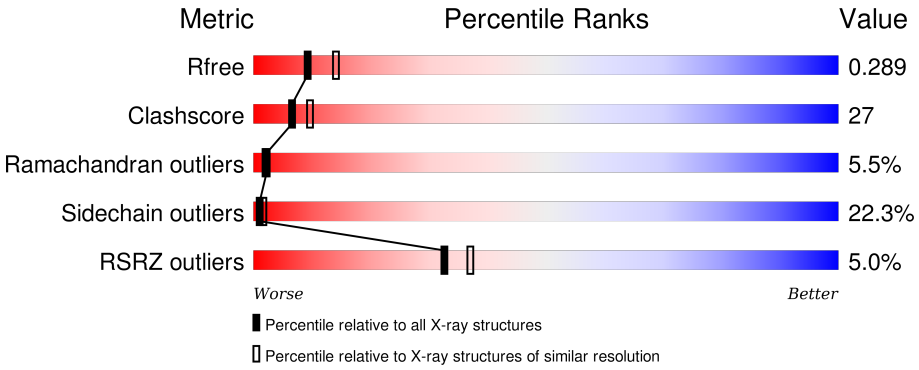
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	3%, 34%, 38%, 19%, 9%
1	B	149	5%, 27%, 47%, 19%, 7%
1	C	149	5%, 35%, 47%, 12%, 6%
1	D	149	7%, 28%, 42%, 21%, 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4917 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
			1119	718	181	219	1			
1	B	149	Total	C	N	O	S	0	0	0
			1118	717	181	219	1			
1	C	149	Total	C	N	O	S	0	0	0
			1126	722	182	221	1			
1	D	149	Total	C	N	O	S	0	0	0
			1123	720	181	221	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 water.

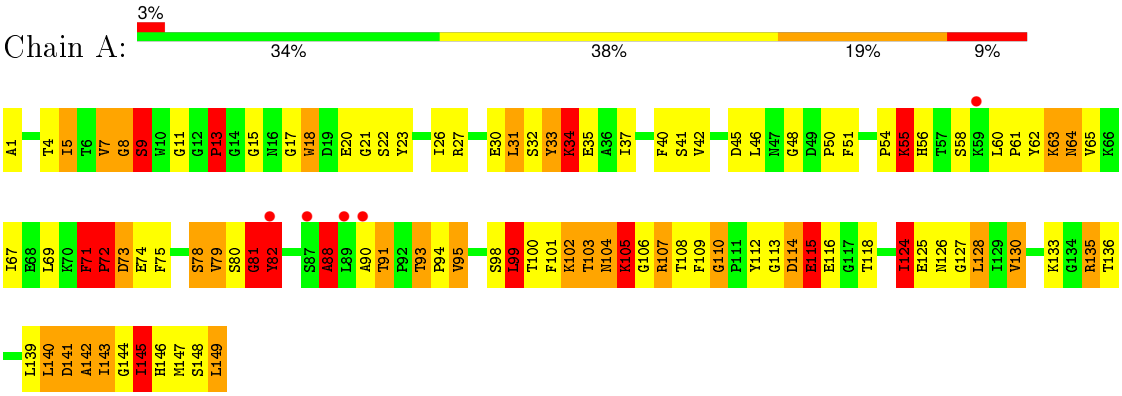
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	102	Total O 102 102	0	0
2	B	112	Total O 112 112	0	0
2	C	105	Total O 105 105	0	0
2	D	112	Total O 112 112	0	0

3 Residue-property plots (i)

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.

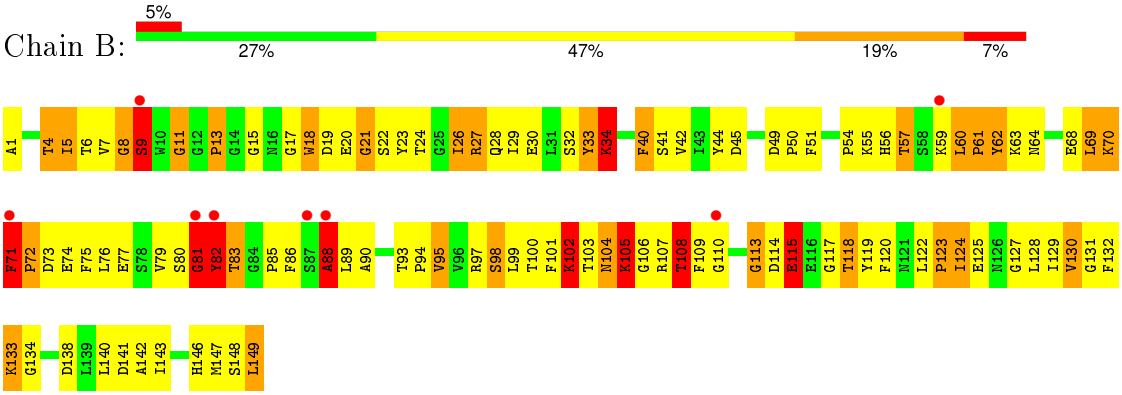
- Molecule 1: Artocarpin

Chain A:



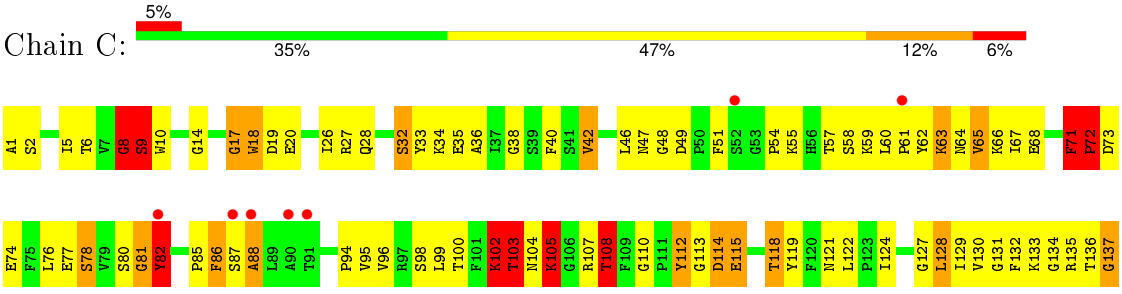
- Molecule 1: Artocarpin

Chain B:

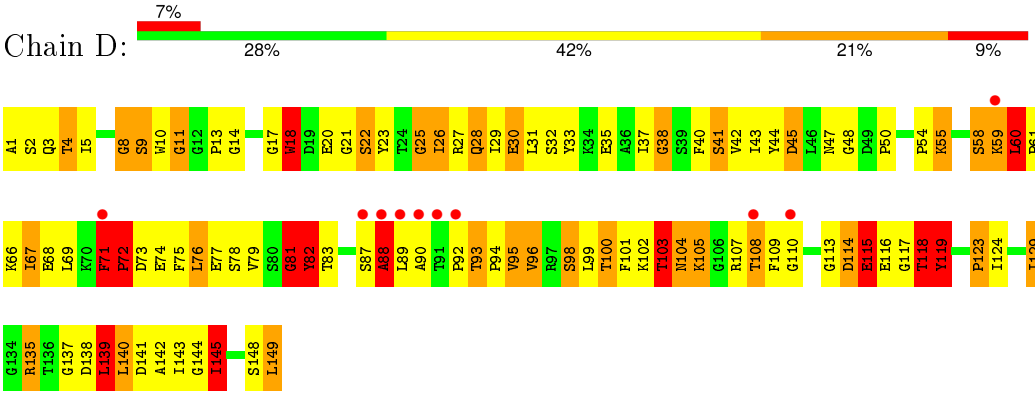


- Molecule 1: Artocarpin

Chain C:



• Molecule 1: Artocarpin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.88Å 73.74Å 60.64Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 10.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 78.9 (10.00-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.262 0.230 , 0.289	Depositor DCC
R_{free} test set	866 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 17578 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4917	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	3.37	3/1149 (0.3%)	2.62	51/1561 (3.3%)
1	B	1.01	3/1149 (0.3%)	2.60	75/1563 (4.8%)
1	C	0.84	2/1157 (0.2%)	2.11	59/1572 (3.8%)
1	D	3.21	2/1153 (0.2%)	2.56	75/1566 (4.8%)
All	All	2.41	10/4608 (0.2%)	2.48	260/6262 (4.2%)

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	1	5
1	B	1	7
1	C	1	5
1	D	1	4
All	All	4	21

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ALA	C-O	109.76	3.31	1.23
1	D	1	ALA	C-O	105.32	3.23	1.23
1	B	70	LYS	C-N	17.96	1.75	1.34
1	A	82	TYR	C-N	-11.34	1.07	1.34
1	D	82	TYR	C-N	-8.24	1.15	1.34
1	B	33	TYR	C-N	6.87	1.49	1.34
1	A	9	SER	C-N	6.51	1.49	1.34
1	B	9	SER	C-N	6.42	1.48	1.34
1	C	81	GLY	C-N	5.96	1.47	1.34
1	C	96	VAL	CA-CB	5.17	1.65	1.54

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	ALA	CA-C-O	-42.77	30.29	120.10
1	D	1	ALA	CA-C-O	-41.92	32.06	120.10
1	A	82	TYR	O-C-N	-31.99	71.51	122.70
1	B	81	GLY	O-C-N	-28.68	76.81	122.70
1	B	71	PHE	C-N-CD	-27.11	60.95	120.60
1	A	81	GLY	O-C-N	-26.71	79.97	122.70
1	B	71	PHE	O-C-N	-24.30	74.93	121.10
1	A	1	ALA	CB-CA-C	22.92	144.48	110.10
1	D	8	GLY	O-C-N	-21.32	88.59	122.70
1	A	1	ALA	N-CA-CB	-21.15	80.49	110.10
1	D	1	ALA	CB-CA-C	21.11	141.77	110.10
1	B	1	ALA	CB-CA-C	20.46	140.80	110.10
1	C	1	ALA	CB-CA-C	18.45	137.78	110.10
1	D	8	GLY	C-N-CA	18.07	166.88	121.70
1	D	1	ALA	N-CA-CB	-17.96	84.95	110.10
1	D	82	TYR	O-C-N	-17.75	94.30	122.70
1	B	34	LYS	O-C-N	-17.30	95.02	122.70
1	B	1	ALA	N-CA-CB	15.38	131.63	110.10
1	D	9	SER	O-C-N	-15.20	98.38	122.70
1	C	1	ALA	N-CA-CB	14.77	130.78	110.10
1	B	81	GLY	C-N-CA	13.87	156.38	121.70
1	B	81	GLY	CA-C-N	13.81	147.57	117.20
1	B	9	SER	O-C-N	13.62	144.50	122.70
1	C	8	GLY	O-C-N	-13.01	101.89	122.70
1	B	82	TYR	O-C-N	12.79	143.16	122.70
1	A	81	GLY	CA-C-N	12.41	144.50	117.20
1	D	8	GLY	CA-C-N	12.02	143.65	117.20
1	C	81	GLY	O-C-N	-11.82	103.79	122.70
1	B	102	LYS	CG-CD-CE	11.60	146.71	111.90
1	B	82	TYR	CA-C-N	-11.49	91.92	117.20
1	B	33	TYR	C-N-CA	-11.29	93.47	121.70
1	A	82	TYR	CA-C-N	10.70	140.73	117.20
1	D	81	GLY	O-C-N	-10.58	105.77	122.70
1	A	9	SER	CA-C-N	-10.37	94.39	117.20
1	C	1	ALA	CA-C-O	-10.23	98.61	120.10
1	C	139	LEU	CA-CB-CG	9.80	137.83	115.30
1	D	82	TYR	CA-C-N	9.76	138.67	117.20
1	D	9	SER	CA-C-N	9.42	137.93	117.20
1	A	71	PHE	C-N-CD	-9.17	100.44	120.60
1	A	1	ALA	N-CA-C	8.89	135.00	111.00
1	C	71	PHE	N-CA-C	8.81	134.78	111.00
1	B	1	ALA	N-CA-C	-8.70	87.52	111.00
1	B	1	ALA	CA-C-O	-8.60	102.04	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	34	LYS	CA-C-N	8.56	136.03	117.20
1	C	1	ALA	CA-C-N	8.44	135.76	117.20
1	D	1	ALA	N-CA-C	8.24	133.24	111.00
1	C	1	ALA	N-CA-C	-8.20	88.86	111.00
1	B	71	PHE	CA-C-N	8.04	139.62	117.10
1	B	9	SER	CA-C-N	-8.01	99.58	117.20
1	C	82	TYR	CA-C-N	-7.61	100.47	117.20
1	B	102	LYS	CB-CG-CD	-7.53	92.03	111.60
1	B	1	ALA	CA-C-N	7.22	133.09	117.20
1	D	139	LEU	CA-CB-CG	7.22	131.90	115.30
1	D	119	TYR	CA-CB-CG	7.21	127.11	113.40
1	C	81	GLY	N-CA-C	7.20	131.10	113.10
1	C	81	GLY	CA-C-N	7.16	132.96	117.20
1	B	82	TYR	C-N-CA	-7.15	103.83	121.70
1	D	72	PRO	CA-N-CD	-7.07	101.61	111.50
1	B	71	PHE	C-N-CA	6.95	151.18	122.00
1	D	71	PHE	O-C-N	-6.76	108.25	121.10
1	D	81	GLY	CA-C-N	6.60	131.73	117.20
1	D	81	GLY	C-N-CA	6.54	138.04	121.70
1	B	81	GLY	N-CA-C	6.48	129.31	113.10
1	D	3	GLN	O-C-N	-6.48	112.33	122.70
1	B	146	HIS	O-C-N	-6.46	112.36	122.70
1	C	133	LYS	O-C-N	-6.45	112.23	123.20
1	D	38	GLY	O-C-N	-6.40	112.45	122.70
1	A	81	GLY	N-CA-C	6.39	129.07	113.10
1	D	71	PHE	C-N-CD	-6.38	106.57	120.60
1	C	129	ILE	N-CA-C	-6.34	93.89	111.00
1	C	102	LYS	CD-CE-NZ	-6.30	97.22	111.70
1	B	98	SER	O-C-N	-6.26	112.69	122.70
1	D	118	THR	O-C-N	-6.23	112.73	122.70
1	C	17	GLY	O-C-N	-6.21	112.77	122.70
1	C	103	THR	O-C-N	-6.18	112.81	122.70
1	B	95	VAL	O-C-N	-6.16	112.84	122.70
1	C	38	GLY	O-C-N	-6.15	112.87	122.70
1	A	17	GLY	O-C-N	-6.11	112.93	122.70
1	A	99	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	C	134	GLY	O-C-N	-6.09	112.96	122.70
1	D	144	GLY	O-C-N	-6.08	112.98	122.70
1	B	113	GLY	O-C-N	-6.07	112.98	122.70
1	C	9	SER	N-CA-C	-6.06	94.63	111.00
1	B	88	ALA	N-CA-C	-6.06	94.64	111.00
1	B	73	ASP	O-C-N	-6.06	113.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	98	SER	O-C-N	-6.05	113.02	122.70
1	A	63	LYS	O-C-N	-6.04	113.03	122.70
1	D	17	GLY	O-C-N	-6.04	113.03	122.70
1	B	117	GLY	O-C-N	-6.03	113.05	122.70
1	D	32	SER	O-C-N	-6.03	113.06	122.70
1	A	80	SER	O-C-N	-6.02	112.97	123.20
1	A	73	ASP	O-C-N	-6.01	113.08	122.70
1	C	5	ILE	O-C-N	-6.01	113.09	122.70
1	D	67	ILE	O-C-N	-5.99	113.11	122.70
1	D	71	PHE	CA-C-N	5.99	133.86	117.10
1	A	95	VAL	O-C-N	-5.99	113.12	122.70
1	B	115	GLU	O-C-N	-5.93	113.21	122.70
1	A	105	LYS	O-C-N	-5.93	113.12	123.20
1	D	108	THR	O-C-N	-5.92	113.23	122.70
1	A	72	PRO	CA-N-CD	-5.92	103.22	111.50
1	D	41	SER	O-C-N	-5.88	113.30	122.70
1	B	17	GLY	O-C-N	-5.86	113.32	122.70
1	B	27	ARG	O-C-N	-5.86	113.33	122.70
1	B	32	SER	O-C-N	-5.86	113.33	122.70
1	B	70	LYS	N-CA-C	-5.85	95.19	111.00
1	A	113	GLY	O-C-N	-5.85	113.34	122.70
1	D	55	LYS	O-C-N	-5.85	113.35	122.70
1	C	34	LYS	O-C-N	-5.83	113.38	122.70
1	C	82	TYR	O-C-N	5.82	132.01	122.70
1	B	108	THR	O-C-N	-5.82	113.39	122.70
1	B	33	TYR	CA-C-N	-5.81	104.41	117.20
1	D	105	LYS	O-C-N	-5.81	113.33	123.20
1	D	54	PRO	O-C-N	-5.80	113.42	122.70
1	D	11	GLY	O-C-N	-5.79	113.37	123.20
1	B	80	SER	O-C-N	-5.78	113.37	123.20
1	C	78	SER	O-C-N	-5.78	113.45	122.70
1	A	64	ASN	O-C-N	-5.77	113.47	122.70
1	D	63	LYS	O-C-N	-5.76	113.49	122.70
1	A	5	ILE	O-C-N	-5.76	113.49	122.70
1	D	50	PRO	O-C-N	-5.75	113.50	122.70
1	B	149	LEU	CA-CB-CG	5.75	128.51	115.30
1	C	95	VAL	O-C-N	-5.74	113.52	122.70
1	D	124	ILE	O-C-N	-5.72	113.55	122.70
1	D	4	THR	O-C-N	-5.70	113.58	122.70
1	C	128	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	34	LYS	O-C-N	-5.69	113.60	122.70
1	B	133	LYS	O-C-N	-5.69	113.53	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	GLU	O-C-N	-5.68	113.61	122.70
1	D	30	GLU	O-C-N	-5.67	113.62	122.70
1	C	6	THR	O-C-N	-5.67	113.63	122.70
1	D	95	VAL	O-C-N	-5.66	113.64	122.70
1	D	100	THR	O-C-N	-5.66	113.65	122.70
1	B	21	GLY	O-C-N	-5.65	113.66	122.70
1	C	137	GLY	O-C-N	-5.65	113.66	122.70
1	D	117	GLY	O-C-N	-5.64	113.68	122.70
1	C	20	GLU	O-C-N	-5.61	113.66	123.20
1	A	31	LEU	O-C-N	-5.61	113.72	122.70
1	D	25	GLY	O-C-N	-5.61	113.72	122.70
1	A	55	LYS	O-C-N	-5.61	113.73	122.70
1	B	123	PRO	O-C-N	-5.61	113.73	122.70
1	C	54	PRO	O-C-N	-5.60	113.74	122.70
1	B	86	PHE	O-C-N	-5.60	113.74	122.70
1	B	64	ASN	O-C-N	-5.56	113.80	122.70
1	B	40	PHE	O-C-N	-5.56	113.81	122.70
1	D	22	SER	O-C-N	-5.56	113.81	122.70
1	A	15	GLY	O-C-N	-5.56	113.81	122.70
1	B	9	SER	CB-CA-C	5.55	120.64	110.10
1	B	4	THR	O-C-N	-5.55	113.82	122.70
1	C	46	LEU	O-C-N	-5.53	113.85	122.70
1	A	135	ARG	O-C-N	-5.53	113.85	122.70
1	D	48	GLY	O-C-N	-5.52	113.87	122.70
1	D	103	THR	O-C-N	-5.51	113.89	122.70
1	A	26	ILE	O-C-N	-5.50	113.90	122.70
1	C	67	ILE	O-C-N	-5.49	113.91	122.70
1	C	113	GLY	O-C-N	-5.48	113.94	122.70
1	A	58	SER	O-C-N	-5.47	113.94	122.70
1	A	107	ARG	O-C-N	-5.47	113.95	122.70
1	D	45	ASP	O-C-N	-5.46	113.96	122.70
1	A	140	LEU	O-C-N	-5.46	113.96	122.70
1	A	124	ILE	O-C-N	-5.46	113.97	122.70
1	C	77	GLU	O-C-N	-5.45	113.97	122.70
1	A	88	ALA	N-CA-C	-5.44	96.31	111.00
1	C	112	TYR	O-C-N	-5.44	113.95	123.20
1	C	115	GLU	O-C-N	-5.44	114.00	122.70
1	C	127	GLY	O-C-N	-5.43	114.01	122.70
1	B	125	GLU	O-C-N	-5.42	114.02	122.70
1	A	78	SER	O-C-N	-5.41	114.04	122.70
1	B	63	LYS	O-C-N	-5.41	114.05	122.70
1	B	106	GLY	O-C-N	-5.40	114.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	131	GLY	O-C-N	-5.40	114.06	122.70
1	B	79	VAL	O-C-N	-5.39	114.07	122.70
1	A	8	GLY	C-N-CA	5.39	135.18	121.70
1	D	10	TRP	O-C-N	-5.38	114.05	123.20
1	C	63	LYS	O-C-N	-5.38	114.09	122.70
1	B	19	ASP	O-C-N	-5.37	114.11	122.70
1	B	26	ILE	O-C-N	-5.37	114.11	122.70
1	B	69	LEU	O-C-N	-5.36	114.12	122.70
1	B	22	SER	O-C-N	-5.35	114.13	122.70
1	D	40	PHE	O-C-N	-5.34	114.15	122.70
1	D	60	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	61	PRO	O-C-N	-5.33	114.17	122.70
1	C	105	LYS	O-C-N	-5.33	114.15	123.20
1	B	118	THR	O-C-N	-5.32	114.18	122.70
1	A	35	GLU	O-C-N	-5.32	114.19	122.70
1	B	68	GLU	O-C-N	-5.32	114.19	122.70
1	D	113	GLY	O-C-N	-5.32	114.19	122.70
1	A	40	PHE	O-C-N	-5.32	114.19	122.70
1	D	99	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	59	LYS	O-C-N	-5.31	114.21	122.70
1	D	47	ASN	O-C-N	-5.30	114.19	123.20
1	D	123	PRO	O-C-N	-5.29	114.24	122.70
1	D	143	ILE	O-C-N	-5.28	114.22	123.20
1	D	14	GLY	O-C-N	-5.28	114.23	123.20
1	A	142	ALA	O-C-N	-5.27	114.26	122.70
1	D	82	TYR	N-CA-C	5.27	125.23	111.00
1	D	129	ILE	O-C-N	-5.27	114.27	122.70
1	B	7	VAL	O-C-N	-5.27	114.25	123.20
1	A	79	VAL	O-C-N	-5.26	114.28	122.70
1	A	145	ILE	O-C-N	-5.26	114.29	122.70
1	B	83	THR	O-C-N	-5.25	114.28	123.20
1	C	85	PRO	O-C-N	-5.24	114.31	122.70
1	D	119	TYR	O-C-N	-5.23	114.34	122.70
1	B	72	PRO	O-C-N	-5.22	114.34	122.70
1	C	19	ASP	O-C-N	-5.22	114.34	122.70
1	C	36	ALA	O-C-N	-5.22	114.34	122.70
1	D	131	GLY	O-C-N	-5.22	114.35	122.70
1	B	13	PRO	O-C-N	-5.21	114.34	123.20
1	D	94	PRO	O-C-N	-5.21	114.36	122.70
1	C	32	SER	O-C-N	-5.21	114.37	122.70
1	C	14	GLY	O-C-N	-5.21	114.35	123.20
1	C	146	HIS	O-C-N	-5.21	114.37	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	ASN	O-C-N	-5.20	114.38	122.70
1	D	18	TRP	O-C-N	-5.20	114.38	122.70
1	D	29	ILE	O-C-N	-5.19	114.39	122.70
1	A	71	PHE	CA-C-N	5.19	131.63	117.10
1	A	82	TYR	C-N-CA	5.17	134.64	121.70
1	C	141	ASP	O-C-N	-5.17	114.42	122.70
1	A	30	GLU	O-C-N	-5.17	114.43	122.70
1	D	77	GLU	O-C-N	-5.17	114.43	122.70
1	C	27	ARG	O-C-N	-5.17	114.43	122.70
1	D	149	LEU	CA-CB-CG	5.16	127.18	115.30
1	B	127	GLY	O-C-N	-5.13	114.49	122.70
1	C	102	LYS	O-C-N	-5.13	114.50	122.70
1	A	149	LEU	CA-CB-CG	5.12	127.09	115.30
1	C	136	THR	O-C-N	-5.12	114.49	123.20
1	D	137	GLY	O-C-N	-5.12	114.51	122.70
1	A	144	GLY	O-C-N	-5.11	114.52	122.70
1	A	33	TYR	O-C-N	-5.11	114.53	122.70
1	C	86	PHE	O-C-N	-5.10	114.54	122.70
1	D	145	ILE	O-C-N	-5.10	114.54	122.70
1	D	65	VAL	O-C-N	-5.09	114.55	122.70
1	B	11	GLY	O-C-N	-5.09	114.55	123.20
1	B	15	GLY	O-C-N	-5.09	114.56	122.70
1	C	10	TRP	O-C-N	-5.08	114.56	123.20
1	C	40	PHE	O-C-N	-5.08	114.57	122.70
1	D	28	GLN	O-C-N	-5.08	114.57	122.70
1	D	43	ILE	O-C-N	-5.08	114.58	122.70
1	B	101	PHE	O-C-N	-5.07	114.58	122.70
1	B	33	TYR	O-C-N	5.07	130.81	122.70
1	C	55	LYS	O-C-N	-5.07	114.59	122.70
1	C	108	THR	O-C-N	-5.07	114.59	122.70
1	C	48	GLY	O-C-N	-5.06	114.60	122.70
1	D	142	ALA	O-C-N	-5.06	114.60	122.70
1	A	71	PHE	O-C-N	-5.05	111.50	121.10
1	B	138	ASP	O-C-N	-5.05	114.61	122.70
1	D	23	TYR	O-C-N	-5.05	114.61	122.70
1	A	32	SER	O-C-N	-5.05	114.62	122.70
1	B	50	PRO	O-C-N	-5.05	114.62	122.70
1	B	62	TYR	O-C-N	-5.05	114.62	122.70
1	B	99	LEU	O-C-N	-5.05	114.62	122.70
1	A	133	LYS	O-C-N	-5.04	114.63	123.20
1	C	57	THR	O-C-N	-5.04	114.64	122.70
1	B	105	LYS	O-C-N	-5.03	114.64	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	76	LEU	O-C-N	-5.03	114.65	122.70
1	D	88	ALA	N-CA-C	-5.02	97.45	111.00
1	B	5	ILE	O-C-N	-5.01	114.69	122.70
1	A	13	PRO	O-C-N	-5.01	114.69	123.20
1	B	85	PRO	O-C-N	-5.01	114.69	122.70
1	D	135	ARG	O-C-N	-5.01	114.69	122.70
1	B	134	GLY	O-C-N	-5.00	114.70	122.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ALA	CA
1	B	1	ALA	CA
1	C	1	ALA	CA
1	D	1	ALA	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ASP	Mainchain
1	A	81	GLY	Mainchain,Peptide
1	A	82	TYR	Mainchain
1	A	9	SER	Mainchain
1	B	109	PHE	Mainchain
1	B	34	LYS	Mainchain
1	B	71	PHE	Mainchain,Peptide
1	B	8	GLY	Peptide
1	B	81	GLY	Mainchain,Peptide
1	C	72	PRO	Mainchain
1	C	8	GLY	Mainchain,Peptide
1	C	9	SER	Mainchain
1	C	94	PRO	Mainchain
1	D	119	TYR	Sidechain
1	D	71	PHE	Mainchain
1	D	8	GLY	Mainchain,Peptide

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	1119	0	1060	73	0
1	B	1118	0	1059	68	0
1	C	1126	0	1076	46	0
1	D	1123	0	1064	65	0
2	A	102	0	0	9	0
2	B	112	0	0	7	0
2	C	105	0	0	6	0
2	D	112	0	0	9	0
All	All	4917	0	4259	239	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.

All (239) 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:B:70:LYS:C	1:B:71:PHE:N	1.75	1.36
1:B:82:TYR:HE2	1:B:115:GLU:HG3	1.10	1.14
1:B:82:TYR:CE2	1:B:115:GLU:HG3	1.92	1.05
1:C:72:PRO:HD3	2:C:171:HOH:O	1.62	0.99
1:A:82:TYR:N	1:A:82:TYR:CD1	2.26	0.99
1:A:55:LYS:HG2	2:A:166:HOH:O	1.66	0.95
1:A:82:TYR:N	1:A:82:TYR:HD1	1.67	0.90
1:A:20:GLU:HG2	1:A:54:PRO:HD2	1.54	0.88
1:A:82:TYR:CE1	1:A:115:GLU:HG3	2.09	0.86
1:A:22:SER:H	1:C:47:ASN:HD21	1.23	0.86
1:B:57:THR:HG23	2:B:170:HOH:O	1.80	0.82
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.44	0.81
1:D:74:GLU:HA	1:D:104:ASN:HD21	1.47	0.80
1:B:20:GLU:HG2	1:B:54:PRO:HD2	1.65	0.78
1:A:23:TYR:O	1:A:130:VAL:HG22	1.83	0.77
1:C:102:LYS:CE	1:C:108:THR:HB	2.14	0.77
1:B:140:LEU:HD21	1:B:143:ILE:HD12	1.66	0.77
1:A:82:TYR:CZ	1:A:115:GLU:HG3	2.21	0.76
1:B:74:GLU:HA	1:B:104:ASN:HD21	1.48	0.76
1:D:78:SER:HB3	1:D:102:LYS:HB2	1.68	0.75
1:B:82:TYR:CE1	1:B:119:TYR:HB2	2.22	0.75
1:C:102:LYS:HE2	1:C:108:THR:HB	1.70	0.73
1:D:11:GLY:HA2	1:D:83:THR:HG21	1.71	0.73
1:C:107:ARG:HD2	2:C:248:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASP:CG	1:D:71:PHE:CE2	2.63	0.72
1:B:103:THR:HG22	1:B:105:LYS:H	1.55	0.71
1:B:45:ASP:OD2	1:B:71:PHE:CE2	2.44	0.71
1:D:74:GLU:OE2	1:D:103:THR:HG21	1.91	0.69
1:B:75:PHE:H	1:B:104:ASN:ND2	1.91	0.69
1:C:8:GLY:HA2	1:D:123:PRO:HD2	1.75	0.68
1:D:45:ASP:CG	1:D:71:PHE:HE2	1.96	0.68
1:B:41:SER:CB	1:B:55:LYS:HD2	2.23	0.68
1:A:27:ARG:HG2	1:A:27:ARG:NH1	2.07	0.68
1:C:74:GLU:OE2	1:C:103:THR:HG21	1.94	0.68
1:A:75:PHE:HA	2:A:158:HOH:O	1.95	0.67
1:A:18:TRP:HH2	1:A:140:LEU:HD13	1.59	0.67
1:A:37:ILE:O	1:A:139:LEU:HB3	1.94	0.67
1:A:9:SER:O	2:A:154:HOH:O	2.13	0.67
1:B:74:GLU:OE2	1:B:103:THR:HG21	1.94	0.66
1:A:74:GLU:OE2	1:A:107:ARG:HD3	1.95	0.66
1:A:41:SER:HB2	1:A:55:LYS:HD2	1.75	0.66
1:C:73:ASP:HB3	1:C:105:LYS:HE2	1.77	0.66
1:D:83:THR:HB	2:D:200:HOH:O	1.96	0.65
1:C:66:LYS:HD2	2:C:240:HOH:O	1.94	0.65
1:D:58:SER:HB2	1:D:138:ASP:O	1.97	0.65
1:D:67:ILE:HG23	1:D:109:PHE:CE2	2.31	0.65
1:D:71:PHE:O	1:D:72:PRO:HG2	1.97	0.65
1:D:129:ILE:HG23	2:D:216:HOH:O	1.96	0.65
1:D:60:LEU:HD23	1:D:139:LEU:HD13	1.78	0.63
1:D:26:ILE:HD12	1:D:26:ILE:N	2.13	0.63
1:B:8:GLY:O	1:B:9:SER:CB	2.48	0.62
1:A:18:TRP:CH2	1:A:140:LEU:HD13	2.35	0.61
1:A:71:PHE:O	1:A:72:PRO:HG2	2.01	0.61
1:A:141:ASP:HB3	2:A:173:HOH:O	1.99	0.60
1:D:95:VAL:HG13	1:D:140:LEU:O	2.01	0.60
1:C:147:MET:HB3	1:D:5:ILE:HD13	1.82	0.60
1:A:98:SER:O	1:A:99:LEU:HB2	2.02	0.60
1:D:71:PHE:CG	1:D:72:PRO:HD2	2.37	0.60
1:A:13:PRO:HD2	1:A:94:PRO:HD2	1.83	0.59
1:A:135:ARG:HG3	1:A:142:ALA:HB3	1.85	0.59
1:B:45:ASP:CG	1:B:71:PHE:CE2	2.77	0.59
1:C:82:TYR:HA	1:C:118:THR:O	2.02	0.58
1:D:135:ARG:HG3	2:D:171:HOH:O	2.02	0.58
1:C:65:VAL:HG11	1:C:112:TYR:CZ	2.39	0.58
1:D:71:PHE:O	1:D:72:PRO:CG	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:OE2	1:A:103:THR:HG21	2.04	0.58
1:C:82:TYR:CE1	1:C:119:TYR:HB2	2.39	0.58
1:A:31:LEU:HD13	1:A:37:ILE:HD12	1.85	0.57
1:D:82:TYR:CE1	1:D:115:GLU:HG3	2.39	0.57
1:C:28:GLN:O	1:C:42:VAL:HG23	2.05	0.57
1:C:103:THR:HG23	1:C:105:LYS:H	1.70	0.56
1:C:102:LYS:HE3	1:C:108:THR:HB	1.86	0.56
1:D:71:PHE:O	1:D:73:ASP:N	2.39	0.56
1:C:98:SER:HB2	1:C:114:ASP:O	2.06	0.56
1:A:103:THR:HB	1:A:107:ARG:O	2.06	0.56
1:C:35:GLU:HA	1:C:114:ASP:OD1	2.06	0.56
1:D:30:GLU:HG3	1:D:66:LYS:HG3	1.87	0.55
1:D:107:ARG:HD2	2:D:190:HOH:O	2.06	0.55
1:D:59:LYS:HE3	2:D:183:HOH:O	2.06	0.55
1:A:71:PHE:CG	1:A:72:PRO:CD	2.90	0.55
1:D:90:ALA:O	1:D:92:PRO:HD3	2.07	0.55
1:C:60:LEU:H	1:C:60:LEU:HD22	1.72	0.55
1:C:74:GLU:HA	1:C:104:ASN:HD21	1.72	0.55
1:D:95:VAL:HG22	1:D:141:ASP:HA	1.88	0.55
1:C:71:PHE:O	1:C:71:PHE:CG	2.60	0.55
1:A:91:THR:HG23	2:A:172:HOH:O	2.07	0.55
1:D:37:ILE:HG13	1:D:96:VAL:HG23	1.89	0.55
1:B:82:TYR:O	1:B:97:ARG:HB2	2.07	0.54
1:C:71:PHE:CD1	1:C:71:PHE:O	2.59	0.54
1:A:23:TYR:CE2	1:A:51:PHE:CD2	2.95	0.54
1:C:108:THR:HG22	2:C:254:HOH:O	2.06	0.54
1:B:128:LEU:HD23	1:D:2:SER:HB3	1.89	0.54
1:B:40:PHE:O	1:B:56:HIS:HB2	2.08	0.54
1:D:35:GLU:HA	1:D:114:ASP:OD1	2.07	0.54
1:D:103:THR:HG23	1:D:105:LYS:H	1.73	0.54
1:B:34:LYS:HD3	1:B:62:TYR:CD1	2.43	0.54
1:A:41:SER:OG	1:A:55:LYS:HE3	2.08	0.54
1:D:67:ILE:HG23	1:D:109:PHE:CD2	2.43	0.53
1:B:76:LEU:HD22	1:B:76:LEU:H	1.74	0.53
1:C:18:TRP:C	1:C:18:TRP:CD1	2.81	0.53
1:A:71:PHE:O	1:A:73:ASP:N	2.41	0.53
1:C:17:GLY:HA2	1:C:135:ARG:HG2	1.90	0.53
1:A:9:SER:HA	1:A:143:ILE:O	2.09	0.53
1:B:123:PRO:HB3	2:B:216:HOH:O	2.08	0.52
1:D:88:ALA:H	1:D:90:ALA:H	1.57	0.52
1:C:103:THR:CG2	1:C:105:LYS:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:SER:HA	1:C:63:LYS:O	2.09	0.52
1:A:71:PHE:CG	1:A:72:PRO:HD2	2.45	0.52
1:D:114:ASP:HB3	2:D:258:HOH:O	2.10	0.52
1:A:48:GLY:HA2	2:A:241:HOH:O	2.09	0.52
1:C:35:GLU:HB2	1:C:86:PHE:CZ	2.44	0.51
1:B:103:THR:CG2	1:B:105:LYS:H	2.22	0.51
1:A:149:LEU:O	1:C:2:SER:HB2	2.11	0.51
1:C:118:THR:HA	2:C:208:HOH:O	2.10	0.51
1:B:114:ASP:HA	2:B:194:HOH:O	2.11	0.51
1:D:133:LYS:HE2	2:D:170:HOH:O	2.09	0.50
1:A:7:VAL:HG23	1:B:124:ILE:CG2	2.42	0.50
1:B:77:GLU:O	1:B:124:ILE:HG12	2.12	0.50
1:A:50:PRO:HD2	2:A:165:HOH:O	2.11	0.50
1:A:74:GLU:HA	1:A:104:ASN:HD21	1.77	0.50
1:B:8:GLY:O	1:B:9:SER:HB3	2.12	0.50
1:D:89:LEU:CB	2:D:249:HOH:O	2.58	0.50
1:A:22:SER:H	1:C:47:ASN:ND2	2.01	0.50
1:A:8:GLY:HA2	1:B:123:PRO:HG2	1.94	0.49
1:A:67:ILE:HG23	1:A:109:PHE:CD2	2.47	0.49
1:B:41:SER:HB3	1:B:55:LYS:HA	1.93	0.49
1:A:34:LYS:HB2	1:A:62:TYR:CD1	2.48	0.49
1:B:59:LYS:HB2	2:B:261:HOH:O	2.11	0.49
1:A:64:ASN:HB3	2:A:167:HOH:O	2.11	0.49
1:D:109:PHE:CD1	1:D:109:PHE:N	2.80	0.49
1:A:71:PHE:CD2	1:A:72:PRO:CD	2.96	0.49
1:A:71:PHE:CB	1:A:72:PRO:HD2	2.42	0.49
1:B:82:TYR:CD2	1:B:115:GLU:HA	2.47	0.49
1:B:41:SER:HB2	1:B:55:LYS:HD2	1.94	0.49
1:B:41:SER:HB3	1:B:55:LYS:HD2	1.93	0.49
1:C:87:SER:O	1:C:88:ALA:HB2	2.13	0.48
1:B:18:TRP:CE2	1:B:56:HIS:CD2	3.02	0.48
1:A:71:PHE:O	1:A:72:PRO:CG	2.62	0.48
1:D:132:PHE:CE1	1:D:145:ILE:HD11	2.49	0.48
1:A:127:GLY:O	1:A:128:LEU:CD1	2.61	0.48
1:B:18:TRP:C	1:B:18:TRP:CD1	2.87	0.47
1:D:75:PHE:H	1:D:104:ASN:ND2	2.12	0.47
1:D:71:PHE:CD2	1:D:72:PRO:HD2	2.50	0.47
1:B:26:ILE:HD13	1:B:129:ILE:O	2.15	0.47
1:B:103:THR:HG22	1:B:105:LYS:N	2.28	0.47
1:A:11:GLY:HA3	1:A:142:ALA:HA	1.97	0.47
1:C:60:LEU:N	1:C:60:LEU:HD22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG23	1:A:146:HIS:N	2.28	0.47
1:B:81:GLY:HA3	1:B:120:PHE:CE2	2.50	0.47
1:B:29:ILE:HG22	1:B:30:GLU:N	2.30	0.47
1:B:81:GLY:O	1:B:98:SER:HB3	2.15	0.47
1:B:21:GLY:HA2	2:B:164:HOH:O	2.15	0.47
1:A:88:ALA:H	1:A:90:ALA:H	1.63	0.46
1:D:41:SER:HB3	1:D:55:LYS:HA	1.96	0.46
1:D:28:GLN:HG3	1:D:68:GLU:HB3	1.97	0.46
1:A:21:GLY:HA3	1:C:47:ASN:ND2	2.29	0.46
1:A:8:GLY:CA	1:B:123:PRO:HG2	2.45	0.46
1:D:45:ASP:CB	1:D:71:PHE:CE2	2.99	0.46
1:A:5:ILE:HD12	1:B:5:ILE:HD12	1.98	0.46
1:D:25:GLY:C	1:D:26:ILE:HD12	2.36	0.46
1:D:81:GLY:O	1:D:98:SER:O	2.34	0.46
1:A:126:ASN:HB3	1:B:6:THR:H	1.81	0.45
1:A:91:THR:OG1	1:A:93:THR:HG23	2.16	0.45
1:B:70:LYS:CA	1:B:71:PHE:N	2.72	0.45
1:D:82:TYR:CE2	1:D:119:TYR:HB2	2.51	0.45
1:D:87:SER:O	1:D:88:ALA:HB2	2.16	0.45
1:D:118:THR:HG22	2:D:248:HOH:O	2.15	0.45
1:A:33:TYR:O	1:A:63:LYS:N	2.48	0.45
1:B:102:LYS:HG3	1:B:108:THR:HB	1.99	0.45
1:D:79:VAL:HG22	1:D:101:PHE:CD2	2.52	0.45
1:A:46:LEU:HD23	1:C:51:PHE:CE2	2.52	0.45
1:A:23:TYR:HE2	1:A:51:PHE:CD2	2.35	0.45
1:B:130:VAL:HG13	1:B:130:VAL:O	2.16	0.45
1:D:38:GLY:C	1:D:58:SER:HB3	2.36	0.45
1:A:124:ILE:HG23	1:A:147:MET:HE1	1.98	0.45
1:C:102:LYS:HE3	1:C:108:THR:CB	2.47	0.45
1:C:132:PHE:CE1	1:C:145:ILE:HD11	2.52	0.45
1:D:60:LEU:HD23	1:D:139:LEU:CD1	2.46	0.44
1:A:79:VAL:HG13	1:A:101:PHE:CE1	2.52	0.44
1:B:27:ARG:CZ	1:B:71:PHE:CD2	3.00	0.44
1:D:33:TYR:CD1	1:D:33:TYR:N	2.85	0.44
1:B:11:GLY:HA3	1:B:142:ALA:HA	1.98	0.44
1:D:44:TYR:OH	1:D:132:PHE:N	2.48	0.44
1:A:127:GLY:O	1:A:128:LEU:HD12	2.17	0.44
1:B:42:VAL:HG11	1:B:132:PHE:HD2	1.82	0.44
1:A:45:ASP:CG	1:A:71:PHE:CE2	2.91	0.44
1:B:45:ASP:OD2	1:B:71:PHE:HE2	1.98	0.44
1:D:71:PHE:CG	1:D:72:PRO:CD	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CD2	1:B:113:GLY:N	2.86	0.44
1:C:121:ASN:ND2	2:C:210:HOH:O	2.50	0.44
1:B:82:TYR:O	1:B:97:ARG:N	2.47	0.44
1:A:18:TRP:O	1:A:18:TRP:CG	2.71	0.44
1:A:71:PHE:CD2	1:A:72:PRO:HD2	2.53	0.44
1:B:33:TYR:HD2	1:B:113:GLY:H	1.63	0.44
1:D:27:ARG:NH1	1:D:27:ARG:HG2	2.33	0.44
1:B:124:ILE:HG21	1:B:147:MET:CE	2.47	0.44
1:C:33:TYR:N	1:C:62:TYR:HB3	2.33	0.44
1:D:45:ASP:HB2	1:D:71:PHE:CE2	2.53	0.43
1:A:78:SER:HB3	1:A:102:LYS:CB	2.47	0.43
1:D:13:PRO:HD2	1:D:93:THR:OG1	2.19	0.43
1:B:42:VAL:HG11	1:B:132:PHE:CD2	2.54	0.43
1:B:60:LEU:HA	1:B:61:PRO:HD3	1.86	0.43
1:B:13:PRO:HD2	1:B:94:PRO:HD2	2.00	0.43
1:C:98:SER:O	1:C:99:LEU:HB2	2.19	0.42
1:A:106:GLY:O	1:A:107:ARG:C	2.57	0.42
1:A:98:SER:HA	1:A:112:TYR:O	2.19	0.42
1:B:27:ARG:CZ	1:B:71:PHE:HD2	2.32	0.42
1:D:26:ILE:CD1	1:D:26:ILE:N	2.83	0.42
1:D:27:ARG:HG2	1:D:27:ARG:HH11	1.85	0.42
1:B:23:TYR:HE2	1:B:51:PHE:CD1	2.37	0.42
1:B:33:TYR:HD2	1:B:113:GLY:N	2.18	0.42
1:C:74:GLU:HA	1:C:104:ASN:ND2	2.35	0.42
1:A:60:LEU:H	1:A:60:LEU:HD22	1.85	0.42
1:D:114:ASP:O	1:D:116:GLU:N	2.50	0.41
1:B:89:LEU:O	1:B:90:ALA:C	2.58	0.41
1:C:80:SER:O	1:C:99:LEU:HD12	2.21	0.41
1:C:33:TYR:H	1:C:62:TYR:HB3	1.86	0.41
1:A:103:THR:HG23	1:A:105:LYS:H	1.84	0.41
1:A:18:TRP:CD1	1:A:56:HIS:NE2	2.88	0.41
1:B:27:ARG:NH1	1:B:71:PHE:HB3	2.36	0.41
1:D:26:ILE:CD1	1:D:129:ILE:HG22	2.51	0.41
1:D:21:GLY:O	1:D:131:GLY:HA3	2.21	0.41
1:A:110:GLY:HA3	2:A:181:HOH:O	2.21	0.41
1:B:34:LYS:HB2	1:B:62:TYR:CD1	2.56	0.41
1:B:88:ALA:H	1:B:90:ALA:H	1.67	0.41
1:A:140:LEU:HD21	1:A:143:ILE:HD12	2.03	0.41
1:C:82:TYR:CZ	1:C:119:TYR:HB2	2.55	0.41
1:D:82:TYR:CD1	1:D:115:GLU:HG3	2.55	0.41
1:B:44:TYR:CE1	1:B:131:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:SER:CB	1:D:55:LYS:HA	2.50	0.41
1:C:122:LEU:HA	1:C:122:LEU:HD12	1.76	0.41
1:B:41:SER:HA	2:B:169:HOH:O	2.20	0.40
1:B:21:GLY:O	1:B:131:GLY:HA3	2.21	0.40
1:B:119:TYR:HB3	2:B:151:HOH:O	2.21	0.40
1:A:60:LEU:HA	1:A:61:PRO:HD3	1.72	0.40
1:A:114:ASP:C	1:A:116:GLU:H	2.25	0.40
1:D:18:TRP:HE1	1:D:20:GLU:HG3	1.86	0.40
1:D:18:TRP:C	1:D:18:TRP:CD1	2.95	0.40
1:C:26:ILE:HD12	1:C:26:ILE:N	2.37	0.40

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	146/149 (98%)	124 (85%)	13 (9%)	9 (6%)	2	1
1	B	147/149 (99%)	130 (88%)	11 (8%)	6 (4%)	3	4
1	C	147/149 (99%)	129 (88%)	9 (6%)	9 (6%)	2	1
1	D	146/149 (98%)	128 (88%)	10 (7%)	8 (6%)	2	2
All	All	586/596 (98%)	511 (87%)	43 (7%)	32 (6%)	2	2

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	72	PRO
1	A	82	TYR
1	A	99	LEU
1	A	110	GLY

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Mol	Chain	Res	Type
1	A	115	GLU
1	B	72	PRO
1	B	115	GLU
1	C	9	SER
1	C	71	PHE
1	C	82	TYR
1	C	88	ALA
1	D	72	PRO
1	D	82	TYR
1	D	115	GLU
1	A	88	ALA
1	B	82	TYR
1	B	110	GLY
1	C	72	PRO
1	C	110	GLY
1	D	71	PHE
1	D	81	GLY
1	D	88	ALA
1	D	110	GLY
1	A	34	LYS
1	B	88	ALA
1	C	81	GLY
1	C	137	GLY
1	C	61	PRO
1	B	9	SER
1	D	61	PRO
1	A	81	GLY

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	117/122 (96%)	88 (75%)	29 (25%)	1 1
1	B	117/122 (96%)	91 (78%)	26 (22%)	1 2
1	C	119/122 (98%)	95 (80%)	24 (20%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	118/122 (97%)	92 (78%)	26 (22%)	1 2
All	All	471/488 (96%)	366 (78%)	105 (22%)	1 2

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	7	VAL
1	A	9	SER
1	A	13	PRO
1	A	18	TRP
1	A	42	VAL
1	A	55	LYS
1	A	65	VAL
1	A	69	LEU
1	A	82	TYR
1	A	91	THR
1	A	93	THR
1	A	95	VAL
1	A	100	THR
1	A	102	LYS
1	A	103	THR
1	A	104	ASN
1	A	105	LYS
1	A	108	THR
1	A	115	GLU
1	A	118	THR
1	A	124	ILE
1	A	128	LEU
1	A	130	VAL
1	A	136	THR
1	A	141	ASP
1	A	143	ILE
1	A	145	ILE
1	A	148	SER
1	B	4	THR
1	B	18	TRP
1	B	24	THR
1	B	28	GLN
1	B	49	ASP
1	B	57	THR
1	B	60	LEU

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	83	THR
1	B	93	THR
1	B	95	VAL
1	B	100	THR
1	B	102	LYS
1	B	104	ASN
1	B	105	LYS
1	B	107	ARG
1	B	108	THR
1	B	115	GLU
1	B	118	THR
1	B	122	LEU
1	B	124	ILE
1	B	130	VAL
1	B	133	LYS
1	B	141	ASP
1	B	148	SER
1	B	149	LEU
1	C	18	TRP
1	C	42	VAL
1	C	49	ASP
1	C	58	SER
1	C	65	VAL
1	C	68	GLU
1	C	76	LEU
1	C	78	SER
1	C	100	THR
1	C	102	LYS
1	C	103	THR
1	C	105	LYS
1	C	108	THR
1	C	114	ASP
1	C	115	GLU
1	C	118	THR
1	C	124	ILE
1	C	128	LEU
1	C	130	VAL
1	C	139	LEU
1	C	143	ILE
1	C	145	ILE
1	C	148	SER

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Mol	Chain	Res	Type
1	C	149	LEU
1	D	4	THR
1	D	9	SER
1	D	18	TRP
1	D	22	SER
1	D	26	ILE
1	D	31	LEU
1	D	42	VAL
1	D	58	SER
1	D	59	LYS
1	D	60	LEU
1	D	69	LEU
1	D	76	LEU
1	D	93	THR
1	D	96	VAL
1	D	100	THR
1	D	103	THR
1	D	104	ASN
1	D	108	THR
1	D	114	ASP
1	D	115	GLU
1	D	118	THR
1	D	139	LEU
1	D	140	LEU
1	D	145	ILE
1	D	148	SER
1	D	149	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	47	ASN
1	A	104	ASN
1	A	121	ASN
1	B	16	ASN
1	B	47	ASN
1	B	104	ASN
1	C	47	ASN
1	C	104	ASN
1	C	121	ASN
1	D	47	ASN

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Mol	Chain	Res	Type
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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	149/149 (100%)	0.27	5 (3%)	49	54	2, 7, 20, 47	0
1	B	149/149 (100%)	0.34	8 (5%)	29	33	2, 9, 28, 51	0
1	C	149/149 (100%)	0.31	7 (4%)	35	40	2, 7, 26, 48	0
1	D	149/149 (100%)	0.42	10 (6%)	21	23	2, 9, 30, 56	0
All	All	596/596 (100%)	0.33	30 (5%)	32	37	2, 8, 27, 56	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	THR	9.6
1	C	91	THR	6.3
1	B	9	SER	5.0
1	B	87	SER	4.9
1	D	90	ALA	4.8
1	D	87	SER	4.4
1	D	88	ALA	4.3
1	C	87	SER	3.9
1	C	88	ALA	3.6
1	C	82	TYR	3.4
1	C	90	ALA	3.2
1	D	89	LEU	3.2
1	D	71	PHE	3.0
1	B	81	GLY	3.0
1	A	89	LEU	2.8
1	A	90	ALA	2.7
1	A	87	SER	2.6
1	D	108	THR	2.6
1	A	59	LYS	2.5
1	B	82	TYR	2.5
1	A	82	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	2.5
1	B	59	LYS	2.5
1	B	110	GLY	2.4
1	C	61	PRO	2.4
1	B	71	PHE	2.3
1	D	110	GLY	2.3
1	D	92	PRO	2.2
1	C	52	SER	2.1
1	D	59	LYS	2.0

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 carbohydrates 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.