



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:49 PM GMT

PDB ID : 1CLP  
Title : CRYSTAL STRUCTURE OF A CALCIUM-INDEPENDENT PHOSPHOLIPASE-LIKE MYOTOXIC PROTEIN FROM BOTHROPS ASPER VENOM  
Authors : Arni, R.K.; Ward, R.J.; Gutierrez, J.M.; Tulinsky, A.  
Deposited on : 1994-09-12  
Resolution : 2.80 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](mailto: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.

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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

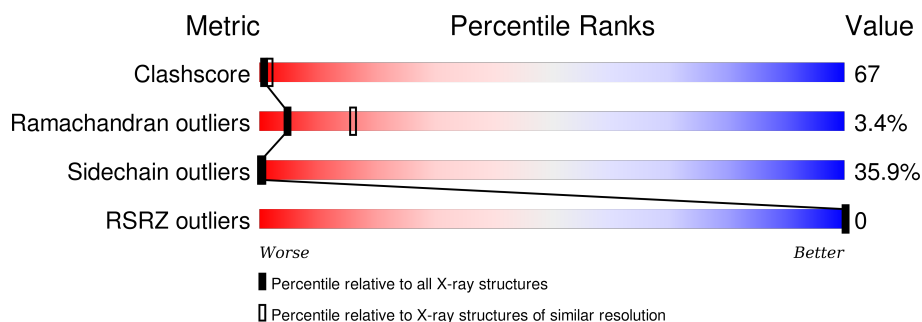
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	121	
1	B	121	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1917 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 MYOTOXIN II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			949	593	166	175	15			
1	B	121	Total	C	N	O	S	0	0	0
			941	586	165	175	15			

- Molecule 2 is water.

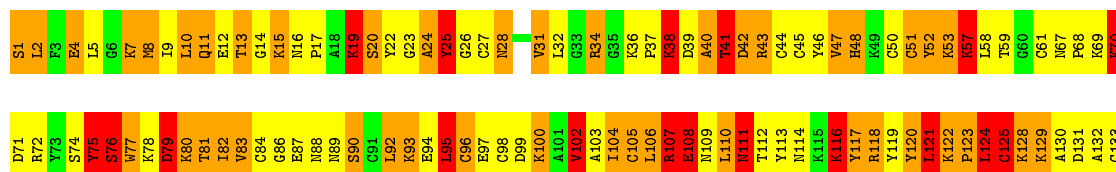
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	11	Total	O	0	0
			11	11		

### 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.

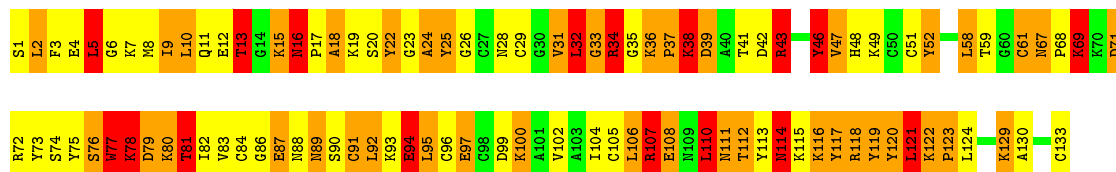
#### • Molecule 1: MYOTOXIN II

Chain A: 



#### • Molecule 1: MYOTOXIN II

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.18Å 67.76Å 88.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80 33.08 – 2.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.80) 72.7 (33.08-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.165 , (Not available) 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 99.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 5805 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	1917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.72	0/966	1.33	4/1292 (0.3%)
1	B	0.68	0/958	1.31	4/1282 (0.3%)
All	All	0.70	0/1924	1.32	8/2574 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	66
1	B	0	59
All	All	0	125

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	77	TRP	CD1-CG-CD2	9.27	113.72	106.30
1	B	77	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	A	77	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	B	77	TRP	CE2-CD2-CG	-7.46	101.34	107.30
1	A	52	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	B	34	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	77	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	B	77	TRP	CB-CG-CD1	-5.29	120.13	127.00

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	102	VAL	Mainchain
1	A	104	ILE	Mainchain
1	A	105	CYS	Mainchain
1	A	107	ARG	Mainchain
1	A	108	GLU	Sidechain,Mainchain
1	A	109	ASN	Mainchain
1	A	11	GLN	Mainchain
1	A	111	ASN	Mainchain
1	A	113	TYR	Mainchain
1	A	116	LYS	Mainchain
1	A	117	TYR	Mainchain
1	A	12	GLU	Mainchain
1	A	120	TYR	Sidechain,Mainchain
1	A	121	LEU	Mainchain
1	A	123	PRO	Mainchain
1	A	124	LEU	Mainchain
1	A	125	CYS	Mainchain
1	A	128	LYS	Mainchain
1	A	132	ALA	Mainchain
1	A	14	GLY	Mainchain
1	A	15	LYS	Mainchain
1	A	17	PRO	Mainchain
1	A	19	LYS	Mainchain
1	A	23	GLY	Mainchain
1	A	24	ALA	Mainchain
1	A	25	TYR	Mainchain
1	A	26	GLY	Mainchain
1	A	28	ASN	Mainchain
1	A	31	VAL	Mainchain
1	A	34	ARG	Mainchain
1	A	38	LYS	Mainchain
1	A	39	ASP	Mainchain
1	A	4	GLU	Mainchain
1	A	40	ALA	Mainchain
1	A	41	THR	Mainchain
1	A	42	ASP	Mainchain
1	A	48	HIS	Mainchain
1	A	5	LEU	Mainchain
1	A	50	CYS	Mainchain
1	A	51	CYS	Mainchain
1	A	57	LYS	Mainchain
1	A	61	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	68	PRO	Mainchain
1	A	7	LYS	Mainchain
1	A	70	LYS	Mainchain
1	A	72	ARG	Mainchain
1	A	74	SER	Mainchain
1	A	75	TYR	Sidechain,Mainchain
1	A	76	SER	Mainchain
1	A	77	TRP	Mainchain
1	A	79	ASP	Mainchain
1	A	8	MET	Mainchain
1	A	82	ILE	Mainchain
1	A	84	CYS	Mainchain
1	A	86	GLY	Mainchain
1	A	92	LEU	Mainchain
1	A	93	LYS	Mainchain
1	A	95	LEU	Mainchain
1	A	96	CYS	Mainchain
1	A	97	GLU	Mainchain
1	A	98	CYS	Mainchain
1	A	99	ASP	Mainchain
1	B	105	CYS	Mainchain
1	B	107	ARG	Mainchain
1	B	108	GLU	Mainchain
1	B	110	LEU	Mainchain
1	B	111	ASN	Mainchain
1	B	114	ASN	Mainchain
1	B	117	TYR	Mainchain
1	B	118	ARG	Sidechain
1	B	119	TYR	Mainchain
1	B	120	TYR	Mainchain
1	B	121	LEU	Mainchain
1	B	123	PRO	Mainchain
1	B	13	THR	Mainchain
1	B	16	ASN	Mainchain
1	B	18	ALA	Mainchain
1	B	20	SER	Mainchain
1	B	22	TYR	Mainchain
1	B	24	ALA	Mainchain
1	B	25	TYR	Sidechain,Mainchain
1	B	29	CYS	Mainchain
1	B	3	PHE	Mainchain
1	B	31	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	B	32	LEU	Mainchain
1	B	33	GLY	Mainchain
1	B	34	ARG	Sidechain,Mainchain
1	B	35	GLY	Mainchain
1	B	36	LYS	Mainchain
1	B	38	LYS	Mainchain
1	B	39	ASP	Mainchain
1	B	41	THR	Mainchain
1	B	42	ASP	Mainchain
1	B	43	ARG	Mainchain
1	B	46	TYR	Mainchain
1	B	47	VAL	Mainchain
1	B	5	LEU	Mainchain
1	B	51	CYS	Mainchain
1	B	52	TYR	Sidechain,Mainchain
1	B	58	LEU	Mainchain
1	B	59	THR	Mainchain
1	B	61	CYS	Mainchain
1	B	67	ASN	Mainchain
1	B	69	LYS	Mainchain
1	B	71	ASP	Mainchain
1	B	73	TYR	Sidechain,Mainchain
1	B	74	SER	Mainchain
1	B	77	TRP	Mainchain
1	B	78	LYS	Mainchain
1	B	81	THR	Mainchain
1	B	84	CYS	Mainchain
1	B	9	ILE	Mainchain
1	B	91	CYS	Mainchain
1	B	94	GLU	Mainchain
1	B	95	LEU	Mainchain
1	B	97	GLU	Mainchain
1	B	99	ASP	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	949	0	940	115	0
1	B	941	0	919	140	0
2	A	16	0	0	3	0
2	B	11	0	0	1	0
All	All	1917	0	1859	251	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 67.

All (251) 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:58:LEU:HD11	1:B:95:LEU:HD13	1.22	1.17
1:A:121:LEU:HD13	1:A:124:LEU:HB2	1.17	1.12
1:B:68:PRO:HA	1:B:95:LEU:HD21	1.37	1.03
1:B:34:ARG:HH11	1:B:34:ARG:HG2	1.24	1.02
1:B:38:LYS:HG2	1:B:117:TYR:HE2	1.29	0.96
1:A:121:LEU:CD1	1:A:124:LEU:HB2	1.95	0.95
1:B:58:LEU:CD1	1:B:95:LEU:HD13	1.96	0.95
1:A:121:LEU:HD13	1:A:124:LEU:CB	1.98	0.93
1:A:36:LYS:HD3	1:A:129:LYS:O	1.67	0.93
1:B:58:LEU:HD22	1:B:61:CYS:SG	2.12	0.88
1:B:16:ASN:ND2	1:B:19:LYS:HB3	1.89	0.87
1:A:111:ASN:HD22	1:A:112:THR:N	1.73	0.87
1:B:10:LEU:HD23	1:B:15:LYS:O	1.73	0.86
1:A:80:LYS:O	1:B:80:LYS:HE2	1.75	0.86
1:A:7:LYS:O	1:A:11:GLN:HG3	1.76	0.85
1:A:13:THR:HG22	1:A:15:LYS:H	1.40	0.85
1:B:1:SER:HB3	1:B:4:GLU:OE1	1.77	0.84
1:A:41:THR:O	1:A:41:THR:HG22	1.78	0.84
1:B:5:LEU:O	1:B:9:ILE:HG13	1.79	0.83
1:A:43:ARG:O	1:A:47:VAL:HG22	1.79	0.82
1:A:107:ARG:HH11	1:A:107:ARG:HB3	1.45	0.82
1:B:118:ARG:HG3	1:B:118:ARG:HH11	1.43	0.81
1:A:121:LEU:HD22	1:A:124:LEU:HD22	1.60	0.81
1:B:34:ARG:HD3	1:B:49:LYS:HB2	1.63	0.81
1:A:37:PRO:HA	1:A:42:ASP:OD2	1.80	0.80
1:B:67:ASN:O	1:B:71:ASP:HB2	1.82	0.80
1:B:67:ASN:HB3	1:B:71:ASP:CG	2.03	0.79
1:B:38:LYS:HG2	1:B:117:TYR:CE2	2.16	0.78
1:B:13:THR:HG23	1:B:15:LYS:HG3	1.66	0.77
1:B:83:VAL:O	1:B:83:VAL:HG23	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:HE2	1:B:116:LYS:HA	1.67	0.75
1:A:120:TYR:HE2	1:A:125:CYS:SG	2.10	0.75
1:A:102:VAL:O	1:A:106:LEU:HB2	1.86	0.74
1:B:107:ARG:HG3	1:B:108:GLU:N	2.01	0.74
1:B:13:THR:HG22	1:B:15:LYS:H	1.51	0.74
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.02	0.73
1:A:31:VAL:HG12	1:A:32:LEU:N	2.03	0.73
1:A:107:ARG:HH11	1:A:107:ARG:CB	2.01	0.73
1:A:111:ASN:HD22	1:A:112:THR:H	1.36	0.72
1:B:15:LYS:O	1:B:17:PRO:HD3	1.90	0.72
1:B:1:SER:HB2	1:B:72:ARG:HG2	1.73	0.70
1:A:36:LYS:HG3	1:A:37:PRO:HD2	1.73	0.70
1:A:58:LEU:HD21	1:A:95:LEU:HB2	1.72	0.70
1:B:82:ILE:HG21	1:B:100:LYS:HB2	1.72	0.70
1:B:13:THR:HG23	1:B:15:LYS:CG	2.21	0.70
1:B:34:ARG:CG	1:B:34:ARG:HH11	2.02	0.69
1:B:78:LYS:HD2	1:B:83:VAL:HG21	1.74	0.69
1:B:58:LEU:HD22	1:B:91:CYS:SG	2.33	0.68
1:B:36:LYS:O	1:B:37:PRO:C	2.30	0.68
1:B:16:ASN:HD21	1:B:19:LYS:CB	2.06	0.67
1:B:116:LYS:HE2	1:B:116:LYS:CA	2.24	0.67
1:A:124:LEU:N	1:A:124:LEU:HD12	2.09	0.67
1:A:31:VAL:HG12	1:A:32:LEU:H	1.60	0.66
1:B:114:ASN:OD1	1:B:116:LYS:HB2	1.96	0.66
1:B:16:ASN:ND2	1:B:19:LYS:CB	2.58	0.66
1:B:114:ASN:HD21	1:B:116:LYS:HB2	1.62	0.65
1:B:93:LYS:O	1:B:97:GLU:HG2	1.97	0.64
1:A:19:LYS:HE3	1:A:119:TYR:OH	1.97	0.64
1:B:114:ASN:ND2	1:B:116:LYS:HB2	2.13	0.64
1:B:89:ASN:HB3	1:B:92:LEU:HB2	1.80	0.64
1:A:124:LEU:N	1:A:124:LEU:CD1	2.61	0.64
1:B:2:LEU:HD22	1:B:69:LYS:HG3	1.78	0.64
1:B:52:TYR:CE2	1:B:68:PRO:HB2	2.32	0.63
1:B:34:ARG:NH1	1:B:34:ARG:HG2	2.05	0.63
1:B:107:ARG:HA	1:B:110:LEU:HB2	1.82	0.61
1:A:9:ILE:O	1:A:13:THR:HB	2.00	0.61
1:A:107:ARG:O	1:A:110:LEU:HB2	2.00	0.61
1:A:36:LYS:HG3	1:A:37:PRO:CD	2.30	0.61
1:A:75:TYR:CD1	1:A:82:ILE:HG23	2.35	0.61
1:A:87:GLU:O	1:A:89:ASN:N	2.32	0.61
1:B:79:ASP:O	1:B:81:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:O	1:A:108:GLU:HB2	2.01	0.60
1:B:1:SER:CB	1:B:72:ARG:HG2	2.31	0.60
1:A:89:ASN:HB3	1:A:92:LEU:HB2	1.83	0.60
1:A:120:TYR:CE2	1:A:125:CYS:SG	2.94	0.60
1:A:25:TYR:CD1	1:A:25:TYR:C	2.74	0.60
1:A:95:LEU:HG	1:A:95:LEU:O	2.02	0.60
1:B:26:GLY:H	1:B:117:TYR:HB3	1.66	0.60
1:A:41:THR:O	1:A:41:THR:CG2	2.49	0.59
1:A:57:LYS:HE3	1:A:58:LEU:CD1	2.32	0.59
1:B:89:ASN:O	1:B:90:SER:HB2	2.02	0.59
1:A:58:LEU:HD12	1:A:94:GLU:OE2	2.02	0.59
1:B:2:LEU:HD22	1:B:69:LYS:CG	2.33	0.59
1:B:122:LYS:CB	1:B:123:PRO:HD3	2.32	0.59
1:A:78:LYS:O	1:A:81:THR:HG23	2.03	0.59
1:A:122:LYS:O	1:A:125:CYS:HB2	2.03	0.58
1:A:43:ARG:HA	1:A:46:TYR:HB3	1.84	0.58
1:B:25:TYR:HE2	1:B:114:ASN:O	1.85	0.58
1:A:34:ARG:NH1	1:A:133:CYS:SG	2.76	0.58
1:B:83:VAL:CG2	1:B:83:VAL:O	2.50	0.57
1:B:25:TYR:HA	1:B:117:TYR:O	2.04	0.57
1:B:28:ASN:O	1:B:49:LYS:HE3	2.05	0.56
1:A:7:LYS:HD3	1:A:75:TYR:OH	2.05	0.56
1:A:22:TYR:CE2	1:A:106:LEU:HG	2.40	0.56
1:B:58:LEU:HD11	1:B:95:LEU:CD1	2.15	0.56
1:A:31:VAL:O	1:A:32:LEU:C	2.44	0.56
1:B:75:TYR:CD1	1:B:75:TYR:C	2.79	0.56
1:A:107:ARG:NH1	1:A:107:ARG:CG	2.66	0.55
1:B:68:PRO:HA	1:B:95:LEU:CD2	2.24	0.55
1:B:8:MET:HE3	1:B:75:TYR:CD2	2.40	0.55
1:B:18:ALA:O	1:B:23:GLY:HA3	2.07	0.55
1:B:75:TYR:CD1	1:B:76:SER:N	2.75	0.54
1:B:34:ARG:HD3	1:B:49:LYS:CB	2.35	0.54
1:A:10:LEU:HD12	1:A:15:LYS:O	2.08	0.54
1:B:46:TYR:CD1	1:B:46:TYR:C	2.79	0.54
1:A:121:LEU:C	1:A:123:PRO:HD2	2.28	0.53
1:B:5:LEU:HD11	1:B:9:ILE:HD11	1.89	0.53
1:A:122:LYS:N	1:A:123:PRO:CD	2.72	0.53
1:B:9:ILE:HG22	1:B:9:ILE:O	2.08	0.53
1:A:102:VAL:HG22	1:A:106:LEU:HD22	1.89	0.53
1:B:114:ASN:HD21	1:B:116:LYS:CB	2.22	0.53
1:A:40:ALA:C	1:A:42:ASP:H	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:HD21	1:A:116:LYS:HB2	1.74	0.52
1:B:114:ASN:CG	1:B:116:LYS:HB2	2.29	0.52
1:B:25:TYR:CD2	1:B:117:TYR:HB2	2.44	0.52
1:A:24:ALA:O	1:A:118:ARG:O	2.27	0.52
1:B:9:ILE:O	1:B:13:THR:HB	2.10	0.52
1:A:44:CYS:SG	1:A:105:CYS:O	2.68	0.52
1:A:80:LYS:HE2	1:B:80:LYS:O	2.10	0.52
1:A:2:LEU:HD21	2:A:359:HOH:O	2.09	0.52
1:A:53:LYS:CB	1:A:53:LYS:NZ	2.73	0.52
1:A:80:LYS:O	1:B:80:LYS:CE	2.54	0.52
1:B:11:GLN:NE2	1:B:75:TYR:OH	2.43	0.52
1:A:25:TYR:HE2	1:A:114:ASN:O	1.93	0.51
1:A:51:CYS:O	1:A:57:LYS:HE2	2.09	0.51
1:A:40:ALA:C	1:A:42:ASP:N	2.64	0.51
1:B:22:TYR:O	1:B:24:ALA:N	2.44	0.51
1:B:9:ILE:HG23	1:B:106:LEU:HD23	1.93	0.51
1:A:22:TYR:HE2	1:A:41:THR:HG23	1.75	0.51
1:B:16:ASN:HD21	1:B:19:LYS:HB2	1.74	0.51
1:A:107:ARG:NH1	1:A:107:ARG:HG2	2.25	0.51
1:A:117:TYR:O	1:A:118:ARG:C	2.47	0.51
1:B:22:TYR:O	1:B:23:GLY:C	2.47	0.51
1:B:31:VAL:O	1:B:33:GLY:N	2.44	0.51
1:A:75:TYR:CD1	1:A:76:SER:N	2.79	0.51
1:B:87:GLU:OE2	1:B:92:LEU:HD23	2.11	0.50
1:B:19:LYS:HE3	1:B:118:ARG:HH21	1.77	0.50
1:B:117:TYR:CD1	1:B:117:TYR:N	2.80	0.50
1:B:34:ARG:O	1:B:129:LYS:HE3	2.12	0.50
1:B:46:TYR:HD1	1:B:46:TYR:C	2.15	0.49
1:B:118:ARG:HH11	1:B:118:ARG:CG	2.14	0.49
1:B:77:TRP:CD1	1:B:77:TRP:O	2.65	0.49
1:A:76:SER:CB	1:A:83:VAL:HG13	2.42	0.49
1:A:79:ASP:O	1:A:81:THR:HG22	2.12	0.49
1:A:2:LEU:CD2	2:A:359:HOH:O	2.60	0.49
1:A:76:SER:HB2	1:A:83:VAL:HG13	1.94	0.49
1:A:31:VAL:CG1	1:A:32:LEU:N	2.73	0.49
1:A:78:LYS:O	1:A:81:THR:CG2	2.60	0.49
1:A:25:TYR:CE2	1:A:114:ASN:O	2.66	0.48
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.77	0.48
1:B:121:LEU:O	1:B:122:LYS:C	2.52	0.48
1:B:61:CYS:N	1:B:91:CYS:SG	2.87	0.48
1:B:87:GLU:HG2	1:B:92:LEU:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLY:O	1:B:17:PRO:HG3	2.14	0.48
1:A:8:MET:HB3	1:A:82:ILE:CD1	2.43	0.48
1:A:121:LEU:HD13	1:A:124:LEU:HD22	1.96	0.48
1:A:20:SER:HB3	1:A:22:TYR:CD1	2.48	0.48
1:A:31:VAL:O	1:A:32:LEU:O	2.32	0.48
1:A:67:ASN:OD1	1:A:70:LYS:HG2	2.14	0.48
1:A:34:ARG:O	1:A:130:ALA:HB2	2.13	0.47
1:A:121:LEU:C	1:A:123:PRO:CD	2.83	0.47
1:A:25:TYR:O	1:A:25:TYR:HD1	1.97	0.47
1:B:114:ASN:HD21	1:B:116:LYS:CG	2.27	0.47
1:B:121:LEU:O	1:B:124:LEU:N	2.42	0.47
1:B:48:HIS:HD2	1:B:102:VAL:HB	1.79	0.47
1:B:82:ILE:CG2	1:B:100:LYS:HD2	2.44	0.47
1:B:25:TYR:CE2	1:B:113:TYR:CE1	3.02	0.47
1:B:5:LEU:CD1	1:B:9:ILE:HD11	2.44	0.47
1:A:8:MET:O	1:A:11:GLN:N	2.47	0.47
1:A:102:VAL:CG1	1:A:103:ALA:N	2.78	0.47
1:B:87:GLU:OE2	1:B:92:LEU:HG	2.15	0.47
1:A:80:LYS:HE3	1:B:12:GLU:OE2	2.15	0.47
1:A:8:MET:HB3	1:A:82:ILE:HD13	1.97	0.46
1:B:13:THR:HG21	1:B:22:TYR:HE2	1.80	0.46
1:B:15:LYS:CE	1:B:110:LEU:HD21	2.45	0.46
1:A:22:TYR:CE2	1:A:41:THR:HG23	2.50	0.46
1:B:107:ARG:O	1:B:110:LEU:HB2	2.16	0.46
1:A:83:VAL:HG22	1:A:83:VAL:O	2.16	0.46
1:A:42:ASP:O	1:A:45:CYS:HB2	2.16	0.46
1:A:48:HIS:O	1:A:48:HIS:CG	2.69	0.46
1:A:31:VAL:CG1	1:A:32:LEU:H	2.27	0.46
1:A:57:LYS:HE3	1:A:58:LEU:HD13	1.97	0.46
1:A:122:LYS:N	1:A:123:PRO:HD3	2.31	0.46
1:A:44:CYS:O	1:A:102:VAL:HG23	2.16	0.45
1:A:25:TYR:CE1	1:A:41:THR:O	2.68	0.45
1:A:28:ASN:OD1	1:A:46:TYR:HD2	1.99	0.45
1:B:67:ASN:HB3	1:B:71:ASP:OD1	2.16	0.45
1:B:26:GLY:N	1:B:117:TYR:HB3	2.32	0.45
1:B:122:LYS:CB	1:B:123:PRO:CD	2.93	0.45
1:B:112:THR:O	1:B:112:THR:HG23	2.16	0.45
1:B:100:LYS:O	1:B:104:ILE:HG13	2.16	0.45
1:A:38:LYS:CE	1:A:38:LYS:HA	2.47	0.45
1:B:94:GLU:O	1:B:97:GLU:HB2	2.17	0.45
1:A:53:LYS:O	1:A:53:LYS:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:O	1:B:89:ASN:ND2	2.48	0.45
1:B:89:ASN:O	1:B:91:CYS:N	2.45	0.44
1:A:79:ASP:CG	1:A:79:ASP:O	2.56	0.44
1:B:8:MET:CE	1:B:75:TYR:CD2	3.00	0.44
1:B:61:CYS:HB3	1:B:91:CYS:HB3	1.78	0.44
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.16	0.44
1:B:31:VAL:HG12	1:B:32:LEU:N	2.32	0.44
1:B:89:ASN:CB	1:B:92:LEU:HB2	2.45	0.44
1:B:38:LYS:CG	1:B:117:TYR:CE2	2.95	0.44
1:A:25:TYR:C	1:A:25:TYR:HD1	2.20	0.44
1:A:90:SER:OG	1:A:90:SER:O	2.35	0.44
1:B:89:ASN:O	1:B:90:SER:CB	2.60	0.44
1:A:122:LYS:HD3	1:A:122:LYS:HA	1.60	0.44
1:B:75:TYR:HD1	1:B:76:SER:N	2.16	0.44
1:A:116:LYS:HD3	1:A:116:LYS:HA	1.68	0.44
1:A:87:GLU:C	1:A:89:ASN:H	2.20	0.44
1:A:38:LYS:HA	1:A:38:LYS:HE3	2.00	0.44
1:B:78:LYS:HB3	1:B:78:LYS:HE2	1.58	0.43
1:B:36:LYS:O	1:B:37:PRO:O	2.34	0.43
1:B:34:ARG:NH2	1:B:133:CYS:SG	2.91	0.43
1:B:75:TYR:HD1	1:B:76:SER:O	2.00	0.43
1:A:1:SER:HB3	1:A:4:GLU:OE1	2.18	0.43
1:A:121:LEU:HD13	1:A:124:LEU:CD2	2.48	0.43
1:B:102:VAL:O	1:B:106:LEU:HD22	2.18	0.43
1:B:107:ARG:CA	1:B:110:LEU:HB2	2.47	0.43
1:B:82:ILE:HG22	1:B:100:LYS:HD2	2.00	0.43
1:B:9:ILE:HD13	1:B:9:ILE:HG21	1.78	0.43
1:B:93:LYS:HG3	1:B:93:LYS:O	2.19	0.43
1:A:13:THR:HG23	1:A:15:LYS:HG3	2.01	0.42
1:B:120:TYR:CD2	1:B:121:LEU:N	2.87	0.42
1:B:69:LYS:HE2	2:B:344:HOH:O	2.19	0.42
1:A:7:LYS:O	1:A:11:GLN:CG	2.58	0.42
1:B:43:ARG:HH11	1:B:43:ARG:HD3	1.67	0.42
1:B:87:GLU:OE2	1:B:92:LEU:CD2	2.68	0.42
1:B:129:LYS:HG3	1:B:130:ALA:H	1.83	0.42
1:A:28:ASN:ND2	1:A:46:TYR:HB2	2.35	0.42
1:B:47:VAL:CG1	1:B:47:VAL:O	2.66	0.42
1:B:118:ARG:HD3	1:B:119:TYR:CZ	2.55	0.42
1:B:118:ARG:HD3	1:B:119:TYR:CE2	2.54	0.42
1:B:15:LYS:HE3	1:B:110:LEU:HD21	2.01	0.42
1:B:36:LYS:HA	1:B:37:PRO:HD2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HG3	1:B:130:ALA:N	2.34	0.41
1:B:114:ASN:C	1:B:116:LYS:N	2.73	0.41
1:B:120:TYR:O	1:B:122:LYS:N	2.53	0.41
1:B:67:ASN:C	1:B:71:ASP:HB2	2.38	0.41
1:A:121:LEU:CD2	1:A:124:LEU:HD22	2.41	0.41
1:A:96:CYS:O	1:A:100:LYS:HB2	2.20	0.41
1:B:107:ARG:C	1:B:110:LEU:HB2	2.41	0.41
1:A:75:TYR:C	1:A:75:TYR:CD1	2.93	0.41
1:B:37:PRO:HD3	1:B:46:TYR:CD2	2.55	0.41
1:B:31:VAL:HG12	1:B:32:LEU:HD13	2.03	0.41
1:B:82:ILE:HB	1:B:100:LYS:HD2	2.03	0.41
1:B:96:CYS:O	1:B:100:LYS:HB3	2.20	0.40
1:A:105:CYS:HB2	2:A:345:HOH:O	2.21	0.40
1:A:123:PRO:HB2	1:A:124:LEU:HD12	2.03	0.40
1:B:102:VAL:C	1:B:104:ILE:N	2.73	0.40
1:A:13:THR:HG22	1:A:15:LYS:N	2.22	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	119/121 (98%)	99 (83%)	18 (15%)	2 (2%)	11	36
1	B	119/121 (98%)	93 (78%)	20 (17%)	6 (5%)	3	8
All	All	238/242 (98%)	192 (81%)	38 (16%)	8 (3%)	5	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	ASP
1	A	128	LYS

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Mol	Chain	Res	Type
1	B	115	LYS
1	B	32	LEU
1	B	37	PRO
1	B	88	ASN
1	A	90	SER
1	B	86	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	104/105 (99%)	61 (59%)	43 (41%)	0	0
1	B	102/105 (97%)	71 (70%)	31 (30%)	0	1
All	All	206/210 (98%)	132 (64%)	74 (36%)	0	0

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	LEU
1	A	10	LEU
1	A	13	THR
1	A	16	ASN
1	A	19	LYS
1	A	20	SER
1	A	25	TYR
1	A	27	CYS
1	A	38	LYS
1	A	41	THR
1	A	43	ARG
1	A	47	VAL
1	A	52	TYR
1	A	53	LYS
1	A	57	LYS
1	A	59	THR

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Mol	Chain	Res	Type
1	A	69	LYS
1	A	70	LYS
1	A	71	ASP
1	A	75	TYR
1	A	76	SER
1	A	79	ASP
1	A	80	LYS
1	A	81	THR
1	A	83	VAL
1	A	88	ASN
1	A	93	LYS
1	A	95	LEU
1	A	102	VAL
1	A	106	LEU
1	A	107	ARG
1	A	108	GLU
1	A	110	LEU
1	A	111	ASN
1	A	116	LYS
1	A	118	ARG
1	A	121	LEU
1	A	122	LYS
1	A	124	LEU
1	A	125	CYS
1	A	129	LYS
1	A	131	ASP
1	B	2	LEU
1	B	5	LEU
1	B	7	LYS
1	B	10	LEU
1	B	13	THR
1	B	15	LYS
1	B	16	ASN
1	B	38	LYS
1	B	39	ASP
1	B	43	ARG
1	B	46	TYR
1	B	69	LYS
1	B	76	SER
1	B	78	LYS
1	B	80	LYS
1	B	81	THR

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	89	ASN
1	B	92	LEU
1	B	94	GLU
1	B	100	LYS
1	B	106	LEU
1	B	107	ARG
1	B	110	LEU
1	B	111	ASN
1	B	112	THR
1	B	114	ASN
1	B	116	LYS
1	B	121	LEU
1	B	122	LYS
1	B	129	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	111	ASN
1	A	114	ASN
1	B	11	GLN
1	B	16	ASN
1	B	48	HIS
1	B	88	ASN
1	B	114	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](#)

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

## 5.5 Carbohydrates [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	121/121 (100%)	-0.69	0 100 100	2, 9, 25, 37	0
1	B	121/121 (100%)	-0.67	0 100 100	2, 12, 26, 35	0
All	All	242/242 (100%)	-0.68	0 100 100	2, 11, 26, 37	0

There are no RSRZ outliers to report.

### 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.