



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:23 PM GMT

PDB ID : 1DPR  
Title : STRUCTURES OF THE APO-AND METAL ION ACTIVATED FORMS  
OF THE DIPHTHERIA TOX REPRESSOR FROM CORYNEBACTERIUM  
DIPHTHERIAE  
Authors : Schiering, N.; Tao, X.; Murphy, J.; Petsko, G.A.; Ringe, D.  
Deposited on : 1995-02-06  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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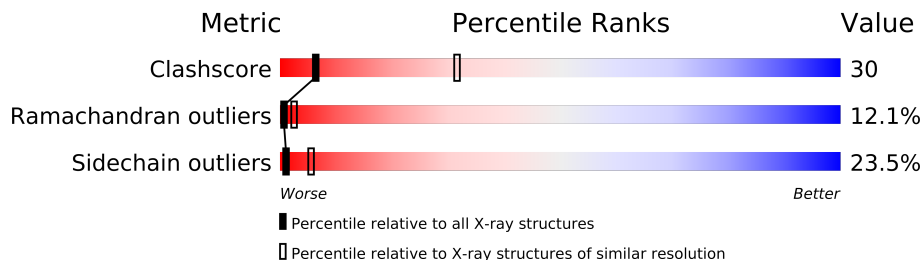
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2122 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DIPHTHERIA TOX REPRESSOR.

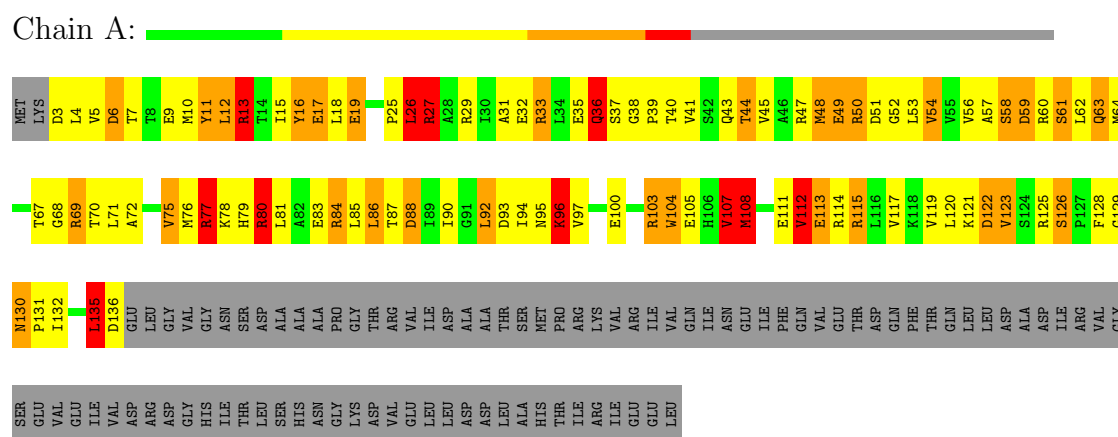
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1061	655	195	205	6			
1	B	134	Total	C	N	O	S	0	0	0
			1061	655	195	205	6			

### 3 Residue-property plots

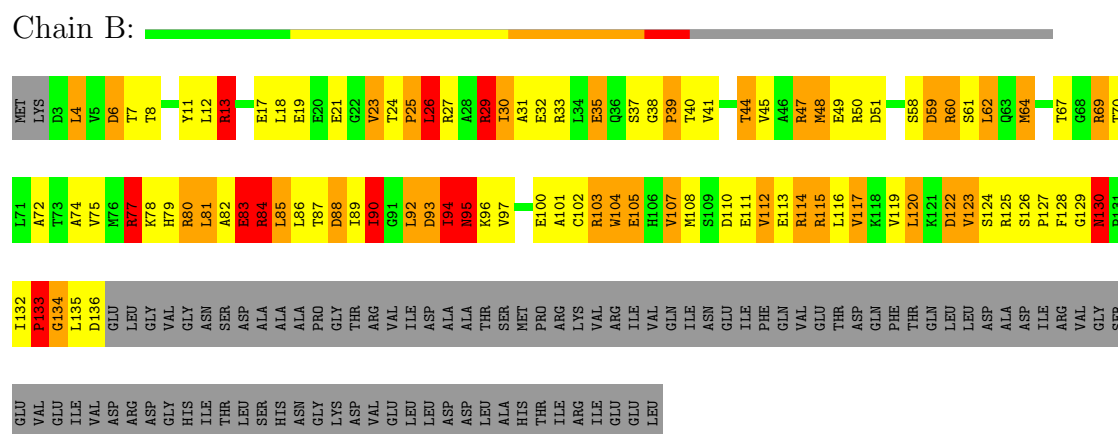
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: DIPHTHERIA TOX REPRESSOR



#### • Molecule 1: DIPHTHERIA TOX REPRESSOR



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.00Å 64.00Å 220.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.241 , 0.417	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

## 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	1.17	2/1074 (0.2%)	2.42	60/1453 (4.1%)
1	B	1.15	0/1074	2.54	72/1453 (5.0%)
All	All	1.16	2/2148 (0.1%)	2.48	132/2906 (4.5%)

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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	SER	CA-CB	7.22	1.63	1.52
1	A	50	ARG	NE-CZ	6.64	1.41	1.33

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	NE-CZ-NH2	-17.58	111.51	120.30
1	B	103	ARG	NE-CZ-NH1	16.47	128.53	120.30
1	A	50	ARG	NE-CZ-NH1	15.37	127.98	120.30
1	B	115	ARG	NE-CZ-NH1	14.98	127.79	120.30
1	A	69	ARG	NE-CZ-NH1	14.26	127.43	120.30
1	B	50	ARG	NE-CZ-NH2	-13.23	113.69	120.30
1	A	69	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	B	115	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	B	50	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	A	47	ARG	NE-CZ-NH2	-12.08	114.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ARG	NE-CZ-NH2	-11.09	114.76	120.30
1	A	33	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	77	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	B	80	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	77	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	77	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	B	13	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	33	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	A	112	VAL	CA-CB-CG2	-9.47	96.70	110.90
1	A	48	MET	CA-CB-CG	9.26	129.04	113.30
1	B	117	VAL	CA-CB-CG2	-9.10	97.25	110.90
1	B	29	ARG	CA-CB-CG	9.03	133.26	113.40
1	B	64	MET	CA-C-N	-8.95	97.52	117.20
1	A	4	LEU	CA-CB-CG	8.81	135.57	115.30
1	A	63	GLN	CA-C-N	-8.79	97.86	117.20
1	B	123	VAL	CB-CA-C	8.67	127.88	111.40
1	A	64	MET	CG-SD-CE	8.41	113.65	100.20
1	A	6	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	115	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	49	GLU	CA-CB-CG	8.21	131.47	113.40
1	B	47	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	77	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	103	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	107	VAL	N-CA-CB	-7.63	94.72	111.50
1	B	47	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	114	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	123	VAL	N-CA-CB	-7.53	94.94	111.50
1	B	104	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	43	GLN	CA-CB-CG	7.45	129.80	113.40
1	B	90	ILE	CG1-CB-CG2	-7.42	95.07	111.40
1	A	112	VAL	CA-CB-CG1	7.42	122.03	110.90
1	B	104	TRP	CG-CD2-CE3	7.29	140.46	133.90
1	B	80	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	19	GLU	CA-CB-CG	7.18	129.19	113.40
1	A	17	GLU	CA-CB-CG	7.13	129.09	113.40
1	A	115	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	84	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	104	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	11	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	A	47	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	80	ARG	CA-CB-CG	-6.83	98.38	113.40
1	B	7	THR	CA-C-N	6.77	132.10	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	LEU	CB-CG-CD1	-6.70	99.60	111.00
1	B	11	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	B	80	ARG	CB-CG-CD	6.64	128.86	111.60
1	A	84	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	123	VAL	N-CA-C	-6.62	93.13	111.00
1	B	26	LEU	N-CA-CB	-6.61	97.18	110.40
1	A	107	VAL	N-CA-C	-6.61	93.15	111.00
1	B	35	GLU	CA-CB-CG	6.59	127.91	113.40
1	B	104	TRP	CD1-CG-CD2	6.55	111.54	106.30
1	B	29	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	35	GLU	N-CA-CB	-6.49	98.93	110.60
1	A	104	TRP	CD1-CG-CD2	6.48	111.48	106.30
1	B	8	THR	CA-CB-CG2	6.46	121.45	112.40
1	A	16	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	B	114	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	103	ARG	CA-CB-CG	-6.30	99.55	113.40
1	A	13	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	88	ASP	N-CA-CB	-6.26	99.33	110.60
1	A	50	ARG	NH1-CZ-NH2	-6.26	112.52	119.40
1	A	107	VAL	CB-CA-C	6.21	123.19	111.40
1	B	83	GLU	CA-CB-CG	6.14	126.92	113.40
1	B	30	ILE	CA-C-N	6.13	130.68	117.20
1	A	3	ASP	N-CA-C	-6.11	94.51	111.00
1	B	35	GLU	CB-CA-C	6.11	122.61	110.40
1	B	27	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	104	TRP	CB-CG-CD1	-6.06	119.12	127.00
1	B	117	VAL	CA-CB-CG1	5.97	119.85	110.90
1	A	50	ARG	CA-CB-CG	5.96	126.52	113.40
1	A	114	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	126	SER	CA-CB-OG	5.92	127.19	111.20
1	A	36	GLN	CA-CB-CG	-5.91	100.40	113.40
1	A	67	THR	N-CA-CB	-5.88	99.13	110.30
1	B	107	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	B	94	ILE	N-CA-C	-5.85	95.20	111.00
1	A	67	THR	CA-C-N	5.84	127.88	116.20
1	A	135	LEU	CA-C-N	-5.71	104.64	117.20
1	B	112	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	B	62	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	130	ASN	N-CA-C	5.61	126.14	111.00
1	A	63	GLN	O-C-N	5.57	131.61	122.70
1	B	26	LEU	CB-CA-C	5.53	120.70	110.20
1	B	11	TYR	CB-CG-CD1	5.50	124.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	PRO	N-CA-C	5.46	126.31	112.10
1	A	29	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	119	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	A	26	LEU	N-CA-C	-5.44	96.32	111.00
1	B	47	ARG	CA-CB-CG	5.43	125.35	113.40
1	B	25	PRO	CA-C-N	-5.43	105.26	117.20
1	A	63	GLN	CA-CB-CG	5.43	125.34	113.40
1	A	87	THR	N-CA-CB	-5.40	100.03	110.30
1	A	108	MET	CG-SD-CE	-5.38	91.58	100.20
1	A	103	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	27	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	6	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	124	SER	CB-CA-C	-5.30	100.02	110.10
1	A	75	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	A	111	GLU	CA-CB-CG	5.28	125.01	113.40
1	B	60	ARG	O-C-N	5.28	131.15	122.70
1	B	112	VAL	CA-CB-CG1	5.27	118.81	110.90
1	B	112	VAL	CA-CB-CG2	-5.27	102.99	110.90
1	B	45	VAL	CB-CA-C	5.27	121.41	111.40
1	A	136	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	B	35	GLU	N-CA-C	-5.25	96.83	111.00
1	A	80	ARG	CB-CG-CD	5.22	125.18	111.60
1	B	32	GLU	CA-CB-CG	5.22	124.88	113.40
1	B	23	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	7	THR	N-CA-CB	5.18	120.15	110.30
1	B	17	GLU	CA-CB-CG	5.17	124.78	113.40
1	B	83	GLU	N-CA-C	-5.16	97.08	111.00
1	A	50	ARG	CD-NE-CZ	5.14	130.80	123.60
1	B	58	SER	N-CA-C	5.14	124.89	111.00
1	A	49	GLU	CA-C-N	5.14	128.51	117.20
1	B	45	VAL	N-CA-CB	-5.10	100.28	111.50
1	B	122	ASP	N-CA-CB	5.09	119.75	110.60
1	A	26	LEU	CB-CG-CD2	5.08	119.64	111.00
1	B	123	VAL	CA-C-N	5.08	128.37	117.20
1	A	126	SER	N-CA-C	-5.07	97.31	111.00
1	B	94	ILE	CA-CB-CG1	-5.05	101.41	111.00
1	B	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	27	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	TYR	Sidechain
1	B	130	ASN	Peptide
1	B	38	GLY	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1061	0	1080	68	0
1	B	1061	0	1080	68	0
All	All	2122	0	2160	129	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:LEU:HB3	1:B:29:ARG:HG2	1.62	0.82
1:A:78:LYS:HG2	1:A:113:GLU:HG2	1.60	0.82
1:A:9:GLU:HG2	1:A:75:VAL:HG21	1.62	0.81
1:B:80:ARG:HB3	1:B:132:ILE:HG12	1.62	0.81
1:A:26:LEU:HD23	1:A:61:SER:HB2	1.64	0.80
1:A:36:GLN:HG2	1:A:40:THR:HG21	1.66	0.78
1:B:112:VAL:HA	1:B:115:ARG:HG2	1.66	0.77
1:B:19:GLU:HA	1:B:60:ARG:NH2	2.03	0.73
1:B:89:ILE:HG22	1:B:90:ILE:HD12	1.71	0.72
1:B:25:PRO:HD2	1:B:60:ARG:HB3	1.72	0.71
1:B:112:VAL:HA	1:B:115:ARG:CG	2.25	0.67
1:B:84:ARG:HG2	1:B:127:PRO:HD3	1.75	0.67
1:B:24:THR:HG22	1:B:60:ARG:HD2	1.76	0.67
1:A:13:ARG:HD3	1:A:105:GLU:OE1	1.95	0.66
1:B:64:MET:HB2	1:B:69:ARG:HH11	1.62	0.65
1:B:77:ARG:HH11	1:B:134:GLY:HA3	1.62	0.65
1:A:86:LEU:HD11	1:A:100:GLU:HG2	1.80	0.64
1:B:108:MET:HE3	1:B:116:LEU:HD12	1.81	0.62
1:B:23:VAL:HG11	1:B:29:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:ALA:HA	1:A:41:VAL:HG21	1.80	0.62
1:B:111:GLU:O	1:B:115:ARG:HG2	1.99	0.62
1:A:77:ARG:NH1	1:A:135:LEU:H	1.98	0.61
1:B:23:VAL:HG11	1:B:29:ARG:NH2	2.16	0.61
1:A:15:ILE:O	1:A:19:GLU:HB2	2.00	0.61
1:A:78:LYS:HD2	1:A:108:MET:O	2.01	0.61
1:B:127:PRO:HG2	1:B:128:PHE:CE1	2.36	0.61
1:A:115:ARG:HH22	1:B:93:ASP:HB2	1.66	0.61
1:B:94:ILE:HG22	1:B:95:ASN:H	1.66	0.60
1:A:54:VAL:HG11	1:A:62:LEU:HD23	1.83	0.60
1:B:19:GLU:HA	1:B:60:ARG:HH21	1.67	0.60
1:A:80:ARG:HG3	1:A:132:ILE:HA	1.83	0.59
1:A:100:GLU:HA	1:A:103:ARG:HH21	1.68	0.58
1:A:49:GLU:HG3	1:A:54:VAL:O	2.04	0.57
1:A:12:LEU:HB3	1:A:72:ALA:HB2	1.85	0.57
1:B:94:ILE:O	1:B:96:LYS:N	2.37	0.57
1:B:24:THR:HB	1:B:60:ARG:HA	1.87	0.56
1:B:114:ARG:HH22	1:B:115:ARG:NH2	2.03	0.56
1:B:78:LYS:HD3	1:B:113:GLU:OE2	2.06	0.55
1:A:104:TRP:O	1:A:108:MET:HB2	2.07	0.55
1:B:114:ARG:HH22	1:B:115:ARG:HH21	1.53	0.55
1:A:45:VAL:HG13	1:A:62:LEU:HD21	1.89	0.55
1:B:24:THR:CG2	1:B:60:ARG:HD2	2.36	0.54
1:A:92:LEU:HD11	1:A:96:LYS:HG2	1.88	0.54
1:B:18:LEU:HD12	1:B:25:PRO:HA	1.89	0.53
1:A:60:ARG:HE	1:A:63:GLN:HE21	1.56	0.53
1:A:76:MET:O	1:A:80:ARG:HG2	2.09	0.52
1:A:18:LEU:HD23	1:A:33:ARG:HH11	1.75	0.52
1:B:44:THR:O	1:B:48:MET:HB2	2.09	0.52
1:B:18:LEU:O	1:B:21:GLU:HB3	2.09	0.52
1:B:127:PRO:HG2	1:B:128:PHE:CD1	2.45	0.52
1:A:37:SER:OG	1:A:39:PRO:HD2	2.10	0.52
1:A:69:ARG:HH11	1:A:69:ARG:HG3	1.75	0.52
1:B:114:ARG:NH2	1:B:115:ARG:HH21	2.08	0.51
1:A:123:VAL:O	1:A:132:ILE:HG21	2.11	0.51
1:A:126:SER:HB2	1:A:130:ASN:O	2.11	0.51
1:A:59:ASP:HB2	1:A:60:ARG:HG3	1.91	0.50
1:A:107:VAL:HG11	1:B:107:VAL:HG21	1.93	0.50
1:A:115:ARG:NH2	1:B:93:ASP:H	2.10	0.49
1:A:80:ARG:NH2	1:A:130:ASN:HB3	2.28	0.49
1:A:107:VAL:HG13	1:B:104:TRP:CD1	2.48	0.48
1:B:37:SER:O	1:B:41:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLU:HB2	1:B:101:ALA:CB	2.44	0.48
1:B:108:MET:CE	1:B:112:VAL:HG12	2.44	0.48
1:A:96:LYS:HD2	1:B:111:GLU:OE2	2.14	0.47
1:A:85:LEU:HG	1:A:90:ILE:HD12	1.96	0.47
1:A:108:MET:SD	1:A:112:VAL:HG12	2.54	0.47
1:B:24:THR:CB	1:B:60:ARG:HA	2.44	0.47
1:A:69:ARG:O	1:A:69:ARG:HG2	2.13	0.47
1:B:12:LEU:HG	1:B:72:ALA:HB2	1.96	0.47
1:B:93:ASP:O	1:B:94:ILE:HB	2.14	0.47
1:B:85:LEU:O	1:B:89:ILE:HB	2.14	0.47
1:B:84:ARG:HH11	1:B:127:PRO:HD3	1.80	0.47
1:B:102:CYS:O	1:B:105:GLU:HG2	2.15	0.47
1:A:38:GLY:HA2	1:A:41:VAL:HB	1.97	0.46
1:A:60:ARG:HD2	1:A:63:GLN:HB3	1.97	0.46
1:A:44:THR:O	1:A:48:MET:HG3	2.16	0.46
1:B:24:THR:CG2	1:B:60:ARG:HA	2.46	0.46
1:B:75:VAL:O	1:B:79:HIS:HB2	2.15	0.46
1:A:70:THR:OG1	1:A:71:LEU:HD22	2.16	0.46
1:A:17:GLU:HB2	1:A:76:MET:HE1	1.98	0.46
1:B:24:THR:HA	1:B:60:ARG:CD	2.46	0.46
1:B:92:LEU:O	1:B:94:ILE:N	2.49	0.46
1:A:113:GLU:O	1:A:117:VAL:HG13	2.15	0.45
1:A:56:VAL:HA	1:A:61:SER:O	2.16	0.45
1:A:80:ARG:HB2	1:A:132:ILE:HD13	1.98	0.45
1:B:111:GLU:HG3	1:B:114:ARG:HH21	1.81	0.45
1:A:115:ARG:NH2	1:B:93:ASP:HB2	2.31	0.45
1:B:24:THR:HA	1:B:60:ARG:HB3	1.99	0.45
1:A:37:SER:O	1:A:41:VAL:HG23	2.17	0.45
1:B:4:LEU:HD21	1:B:47:ARG:HD3	1.98	0.45
1:B:77:ARG:O	1:B:81:LEU:HB2	2.17	0.45
1:A:53:LEU:HD22	1:A:68:GLY:HA2	2.00	0.44
1:B:77:ARG:NH1	1:B:134:GLY:HA3	2.32	0.44
1:A:18:LEU:HD23	1:A:33:ARG:NH1	2.32	0.44
1:A:57:ALA:N	1:A:63:GLN:OE1	2.51	0.44
1:B:78:LYS:HB2	1:B:78:LYS:HE2	1.85	0.44
1:A:80:ARG:CZ	1:A:130:ASN:HB3	2.48	0.44
1:A:75:VAL:O	1:A:79:HIS:HB2	2.17	0.43
1:A:92:LEU:HB3	1:A:97:VAL:HG23	2.00	0.43
1:B:82:ALA:O	1:B:86:LEU:HG	2.18	0.43
1:B:88:ASP:CG	1:B:120:LEU:HD21	2.38	0.43
1:A:84:ARG:HB3	1:A:120:LEU:HD13	2.01	0.43
1:B:74:ALA:HA	1:B:77:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ARG:NH1	1:A:135:LEU:N	2.64	0.43
1:A:107:VAL:HG22	1:B:103:ARG:HB3	2.00	0.43
1:B:126:SER:O	1:B:129:GLY:N	2.52	0.43
1:A:84:ARG:O	1:A:88:ASP:HB2	2.19	0.43
1:B:30:ILE:O	1:B:33:ARG:HB2	2.18	0.43
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.43
1:B:108:MET:HE3	1:B:112:VAL:HG12	2.01	0.43
1:B:110:ASP:O	1:B:113:GLU:HB2	2.19	0.43
1:A:128:PHE:O	1:A:130:ASN:N	2.51	0.42
1:A:130:ASN:HA	1:A:131:PRO:HD3	1.98	0.42
1:A:86:LEU:HB3	1:A:97:VAL:HG22	2.02	0.42
1:A:11:TYR:OH	1:A:41:VAL:HG22	2.19	0.42
1:B:21:GLU:CD	1:B:33:ARG:HH21	2.23	0.42
1:A:79:HIS:O	1:A:83:GLU:HG3	2.20	0.41
1:B:84:ARG:O	1:B:88:ASP:N	2.53	0.41
1:A:69:ARG:HG3	1:A:69:ARG:NH1	2.33	0.41
1:A:76:MET:SD	1:A:79:HIS:HD2	2.44	0.41
1:A:107:VAL:HG12	1:A:108:MET:H	1.86	0.41
1:B:25:PRO:O	1:B:62:LEU:HG	2.20	0.41
1:B:94:ILE:HA	1:B:94:ILE:HD13	1.97	0.41
1:B:128:PHE:N	1:B:128:PHE:CD1	2.88	0.41
1:A:77:ARG:HB3	1:A:77:ARG:HE	1.78	0.41
1:A:5:VAL:HG23	1:A:6:ASP:N	2.36	0.41
1:A:107:VAL:CG1	1:A:108:MET:H	2.34	0.40
1:A:6:ASP:HA	1:A:9:GLU:HB2	2.01	0.40
1:B:13:ARG:NH2	1:B:102:CYS:SG	2.94	0.40

There are no symmetry-related clashes.

## 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	132/226 (58%)	106 (80%)	12 (9%)	14 (11%)	1	3
1	B	132/226 (58%)	100 (76%)	14 (11%)	18 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	264/452 (58%)	206 (78%)	26 (10%)	32 (12%)	<b>1</b> <b>2</b>

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	58	SER
1	A	92	LEU
1	A	94	ILE
1	A	122	ASP
1	A	135	LEU
1	B	39	PRO
1	B	59	ASP
1	B	84	ARG
1	B	93	ASP
1	B	94	ILE
1	B	95	ASN
1	B	97	VAL
1	B	122	ASP
1	B	133	PRO
1	A	27	ARG
1	A	61	SER
1	A	86	LEU
1	A	93	ASP
1	A	129	GLY
1	B	31	ALA
1	B	70	THR
1	B	134	GLY
1	A	96	LYS
1	A	107	VAL
1	B	69	ARG
1	B	105	GLU
1	A	52	GLY
1	B	61	SER
1	B	123	VAL
1	B	4	LEU
1	B	130	ASN

### 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	119/198 (60%)	92 (77%)	27 (23%)	1	6
1	B	119/198 (60%)	90 (76%)	29 (24%)	1	5
All	All	238/396 (60%)	182 (76%)	56 (24%)	1	5

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	12	LEU
1	A	13	ARG
1	A	25	PRO
1	A	26	LEU
1	A	27	ARG
1	A	32	GLU
1	A	36	GLN
1	A	44	THR
1	A	50	ARG
1	A	51	ASP
1	A	54	VAL
1	A	59	ASP
1	A	77	ARG
1	A	80	ARG
1	A	88	ASP
1	A	95	ASN
1	A	96	LYS
1	A	107	VAL
1	A	108	MET
1	A	112	VAL
1	A	113	GLU
1	A	119	VAL
1	A	121	LYS
1	A	122	ASP
1	A	123	VAL
1	A	125	ARG
1	B	6	ASP
1	B	13	ARG
1	B	26	LEU
1	B	29	ARG
1	B	35	GLU
1	B	39	PRO

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Mol	Chain	Res	Type
1	B	40	THR
1	B	44	THR
1	B	48	MET
1	B	51	ASP
1	B	59	ASP
1	B	67	THR
1	B	77	ARG
1	B	81	LEU
1	B	83	GLU
1	B	85	LEU
1	B	87	THR
1	B	90	ILE
1	B	92	LEU
1	B	94	ILE
1	B	95	ASN
1	B	100	GLU
1	B	117	VAL
1	B	120	LEU
1	B	125	ARG
1	B	130	ASN
1	B	133	PRO
1	B	135	LEU
1	B	136	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	79	HIS
1	A	95	ASN
1	A	98	HIS
1	B	95	ASN
1	B	106	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.