



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:04 PM UTC

PDB ID : 1DPR / pdb_00001dpr
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

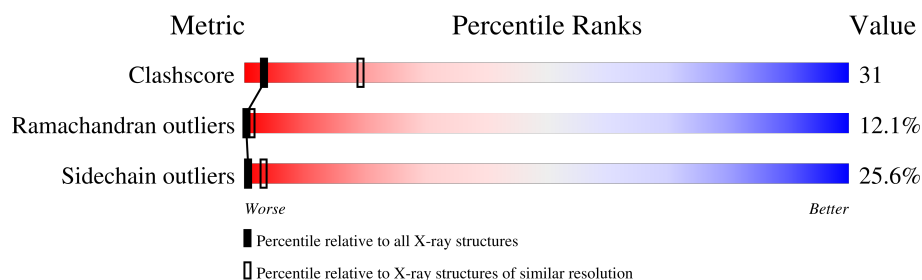
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

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 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 DIPHTHERIA TOX REPRESSOR.

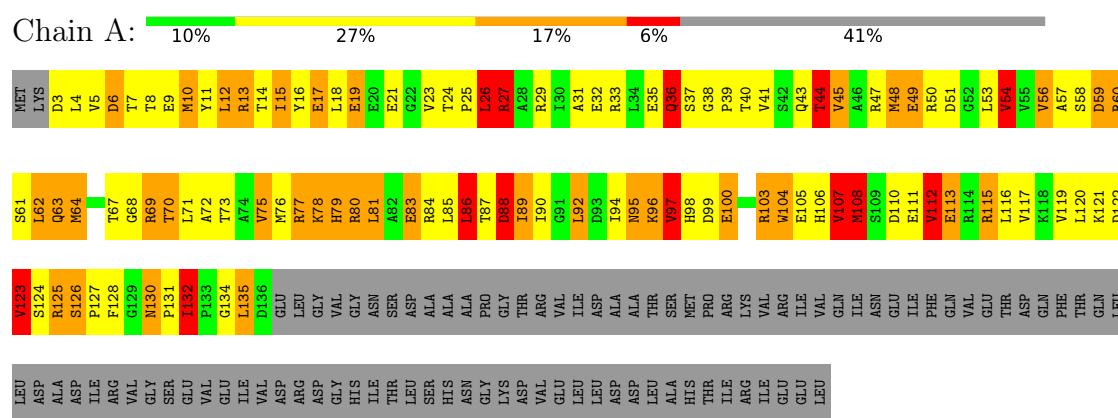
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1061	655	195	205	6			
1	B	134	Total	C	N	O	S	0	0	0
			1061	655	195	205	6			

3 Residue-property plots [i](#)

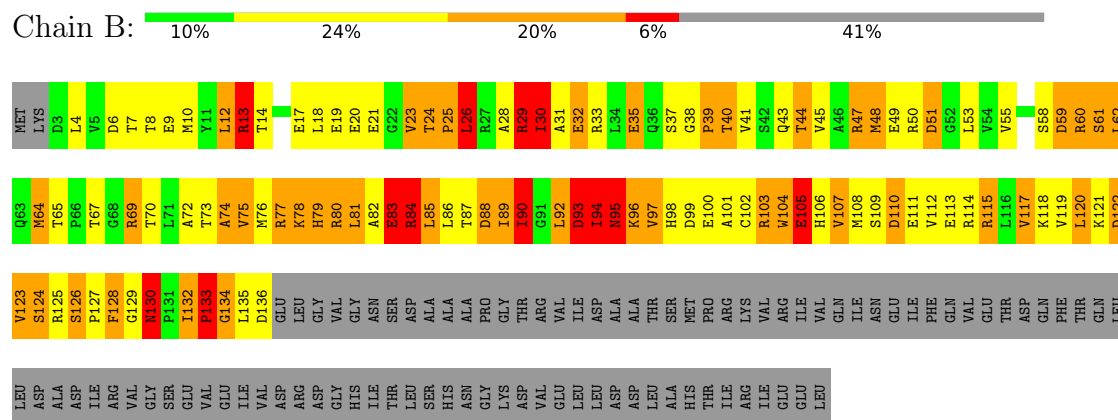
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.00 Å 64.00 Å 220.40 Å 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 ²)	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	1.57	11/1074 (1.0%)	2.69	106/1453 (7.3%)
1	B	1.56	10/1074 (0.9%)	2.75	116/1453 (8.0%)
All	All	1.56	21/2148 (1.0%)	2.72	222/2906 (7.6%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CA-CB	8.32	1.63	1.54
1	A	132	ILE	CA-C	8.01	1.61	1.52
1	B	106	HIS	CD2-NE2	-7.99	1.29	1.37
1	A	50	ARG	NE-CZ	7.85	1.41	1.33
1	B	30	ILE	CA-CB	7.84	1.63	1.54
1	A	132	ILE	CA-CB	7.70	1.64	1.54
1	B	40	THR	CA-CB	7.47	1.65	1.53
1	B	73	THR	CA-CB	7.24	1.64	1.53
1	B	94	ILE	CA-CB	7.09	1.64	1.54
1	A	79	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	94	ILE	CA-CB	6.75	1.63	1.54
1	A	106	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	79	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	58	SER	CA-CB	6.10	1.63	1.53
1	A	95	ASN	CA-CB	6.03	1.60	1.52
1	B	8	THR	CA-CB	5.52	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLN	CA-CB	5.47	1.60	1.52
1	B	20	GLU	CA-CB	-5.39	1.44	1.53
1	B	106	HIS	CG-ND1	-5.30	1.32	1.38
1	B	79	HIS	CG-ND1	-5.23	1.32	1.38
1	A	98	HIS	CD2-NE2	-5.22	1.32	1.37

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASP	CA-CB-CG	11.23	123.83	112.60
1	A	6	ASP	CA-CB-CG	11.14	123.74	112.60
1	B	123	VAL	CB-CA-C	10.11	127.88	111.29
1	A	107	VAL	N-CA-CB	-10.01	94.72	111.23
1	B	123	VAL	N-CA-CB	-9.87	94.94	111.23
1	B	29	ARG	CA-CB-CG	9.58	133.26	114.10
1	B	51	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	112	VAL	N-CA-C	8.81	120.60	111.00
1	A	29	ARG	N-CA-C	-8.80	101.64	111.14
1	B	30	ILE	CA-C-O	-8.78	111.31	121.05
1	B	49	GLU	CA-CB-CG	8.68	131.47	114.10
1	A	126	SER	N-CA-C	-8.68	97.31	110.50
1	B	103	ARG	NE-CZ-NH2	-8.54	111.51	119.20
1	B	7	THR	N-CA-C	-8.46	101.28	111.69
1	B	64	MET	CA-C-O	8.39	130.25	120.69
1	B	7	THR	CA-C-O	-8.26	111.07	120.24
1	B	32	GLU	N-CA-C	-8.18	103.83	113.88
1	B	26	LEU	N-CA-CB	-8.12	97.18	110.42
1	B	35	GLU	N-CA-CB	-8.12	98.93	110.46
1	A	112	VAL	CA-CB-CG2	-8.06	96.70	110.40
1	A	126	SER	CA-CB-OG	8.04	127.19	111.10
1	A	115	ARG	N-CA-C	-8.02	102.12	112.23
1	B	128	PHE	N-CA-C	-8.02	104.47	112.97
1	A	44	THR	N-CA-C	8.00	119.78	111.14
1	B	80	ARG	CA-CB-CG	-7.86	98.38	114.10
1	A	43	GLN	CA-CB-CG	7.85	129.80	114.10
1	B	123	VAL	N-CA-C	-7.79	93.13	109.34
1	A	107	VAL	N-CA-C	-7.78	93.15	109.34
1	B	117	VAL	CA-CB-CG2	-7.74	97.25	110.40
1	A	10	MET	N-CA-C	-7.69	103.86	113.55
1	B	80	ARG	CB-CG-CD	7.63	128.86	111.30
1	B	74	ALA	N-CA-C	7.58	119.24	110.97
1	A	116	LEU	N-CA-C	7.54	119.50	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLU	CA-CB-CG	7.54	129.19	114.10
1	B	88	ASP	N-CA-C	7.54	120.46	111.33
1	A	17	GLU	CA-CB-CG	7.50	129.09	114.10
1	A	48	MET	CA-CB-CG	7.47	129.04	114.10
1	A	26	LEU	N-CA-C	-7.42	96.32	108.41
1	A	63	GLN	CA-C-O	7.41	130.47	120.47
1	A	130	ASN	N-CA-C	7.39	126.14	109.81
1	A	103	ARG	CA-CB-CG	-7.28	99.55	114.10
1	A	107	VAL	CB-CA-C	7.26	123.19	111.29
1	B	76	MET	CA-C-O	-7.17	113.31	120.70
1	B	88	ASP	N-CA-CB	-7.15	99.33	110.06
1	A	67	THR	N-CA-CB	-7.14	99.13	110.19
1	B	95	ASN	CB-CG-ND2	7.09	127.03	116.40
1	A	21	GLU	CB-CG-CD	7.09	124.65	112.60
1	B	103	ARG	NE-CZ-NH1	7.03	128.53	121.50
1	B	132	ILE	CA-C-N	7.03	128.62	119.84
1	B	132	ILE	C-N-CA	7.03	128.62	119.84
1	B	35	GLU	CA-CB-CG	6.90	127.91	114.10
1	A	36	GLN	CA-CB-CG	-6.85	100.40	114.10
1	A	112	VAL	CA-CB-CG1	6.84	122.03	110.40
1	B	94	ILE	N-CA-C	-6.80	95.20	109.34
1	B	35	GLU	CB-CA-C	6.79	122.61	111.41
1	B	94	ILE	CA-C-O	-6.78	112.30	120.78
1	B	107	VAL	N-CA-C	-6.78	106.04	113.43
1	B	97	VAL	N-CA-C	6.72	123.31	109.34
1	B	133	PRO	N-CA-C	6.72	126.31	112.47
1	A	97	VAL	N-CA-C	6.66	119.37	111.05
1	A	7	THR	N-CA-CB	6.64	120.15	110.26
1	A	24	THR	CA-C-N	6.63	128.12	119.84
1	A	24	THR	C-N-CA	6.63	128.12	119.84
1	A	63	GLN	O-C-N	6.62	131.61	123.14
1	B	58	SER	N-CA-C	6.62	124.89	110.80
1	B	60	ARG	CA-C-N	6.57	134.08	121.54
1	B	60	ARG	C-N-CA	6.57	134.08	121.54
1	B	104	TRP	CG-CD2-CE3	6.56	140.46	133.90
1	B	64	MET	N-CA-C	-6.54	99.36	109.76
1	B	60	ARG	O-C-N	6.50	131.15	122.43
1	B	26	LEU	CB-CA-C	6.49	120.70	110.19
1	A	50	ARG	NE-CZ-NH1	6.48	127.98	121.50
1	B	53	LEU	CA-C-O	6.47	125.89	118.97
1	A	123	VAL	CA-C-O	-6.46	111.34	119.48
1	B	8	THR	CA-CB-CG2	6.44	121.45	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	HIS	N-CA-C	6.43	121.41	113.50
1	B	64	MET	O-C-N	6.41	130.54	123.04
1	B	83	GLU	CA-CB-CG	6.41	126.92	114.10
1	B	88	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	61	SER	CA-C-O	-6.32	111.47	120.51
1	B	75	VAL	CA-C-N	6.32	129.04	120.44
1	B	75	VAL	C-N-CA	6.32	129.04	120.44
1	B	115	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	A	132	ILE	N-CA-CB	-6.27	102.43	111.21
1	B	130	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	14	THR	CA-CB-OG1	-6.25	100.22	109.60
1	A	50	ARG	CA-CB-CG	6.21	126.52	114.10
1	B	121	LYS	N-CA-C	-6.18	102.09	110.68
1	B	35	GLU	N-CA-C	-6.13	96.83	108.17
1	B	50	ARG	NE-CZ-NH2	-6.13	113.69	119.20
1	B	12	LEU	CA-C-O	6.07	126.84	119.38
1	B	64	MET	N-CA-CB	6.06	119.34	109.95
1	B	94	ILE	CA-CB-CG2	6.06	120.80	110.50
1	A	36	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	69	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	B	110	ASP	CA-C-O	-6.04	114.44	120.90
1	A	58	SER	CA-CB-OG	6.04	123.18	111.10
1	A	80	ARG	CB-CG-CD	6.03	125.18	111.30
1	B	43	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	B	94	ILE	CB-CA-C	5.99	121.12	111.29
1	A	78	LYS	N-CA-C	-5.99	105.94	113.18
1	A	92	LEU	N-CA-C	5.94	123.45	110.80
1	A	69	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	23	VAL	O-C-N	-5.92	115.17	122.57
1	A	36	GLN	CG-CD-NE2	5.89	125.24	116.40
1	A	3	ASP	N-CA-C	-5.89	94.51	111.00
1	A	124	SER	N-CA-C	5.89	120.31	113.18
1	A	27	ARG	N-CA-C	5.87	123.30	110.80
1	A	122	ASP	CA-CB-CG	-5.87	106.73	112.60
1	B	43	GLN	CA-C-O	5.86	126.63	120.42
1	A	110	ASP	CA-CB-CG	-5.85	106.75	112.60
1	A	83	GLU	CA-C-O	5.82	126.59	120.42
1	A	88	ASP	CA-C-O	-5.82	114.71	120.82
1	A	64	MET	CG-SD-CE	5.80	113.65	100.90
1	B	106	HIS	CA-C-O	5.79	125.35	118.69
1	B	23	VAL	N-CA-C	5.79	117.69	108.89
1	B	124	SER	N-CA-C	5.78	123.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	8	THR	CA-CB-OG1	-5.78	100.94	109.60
1	A	110	ASP	CA-C-N	5.77	128.28	120.38
1	A	110	ASP	C-N-CA	5.77	128.28	120.38
1	B	93	ASP	N-CA-C	5.76	123.08	110.80
1	B	28	ALA	CA-C-N	5.75	128.31	120.54
1	B	28	ALA	C-N-CA	5.75	128.31	120.54
1	A	79	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	A	99	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	115	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	A	75	VAL	N-CA-CB	-5.72	100.87	110.65
1	B	13	ARG	CA-C-O	-5.69	115.04	120.90
1	B	105	GLU	O-C-N	-5.68	115.03	122.59
1	A	127	PRO	N-CA-C	-5.63	105.42	113.47
1	B	47	ARG	CA-CB-CG	5.63	125.35	114.10
1	A	69	ARG	CA-CB-CG	-5.62	102.86	114.10
1	A	63	GLN	CA-CB-CG	5.62	125.34	114.10
1	A	7	THR	N-CA-C	-5.59	104.68	112.45
1	A	23	VAL	N-CA-CB	-5.57	102.04	111.23
1	B	119	VAL	O-C-N	-5.56	116.78	122.23
1	B	117	VAL	CA-CB-CG1	5.56	119.85	110.40
1	B	62	LEU	N-CA-C	5.56	122.64	110.80
1	B	78	LYS	CA-C-N	5.54	128.16	120.29
1	B	78	LYS	C-N-CA	5.54	128.16	120.29
1	A	87	THR	CB-CA-C	5.54	119.58	110.83
1	A	103	ARG	O-C-N	5.54	129.44	122.19
1	A	67	THR	CB-CA-C	5.51	120.64	110.56
1	A	4	LEU	CA-CB-CG	5.51	135.57	116.30
1	A	47	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	B	122	ASP	N-CA-CB	5.48	119.75	110.49
1	A	89	ILE	O-C-N	-5.46	116.74	122.20
1	A	111	GLU	CA-CB-CG	5.46	125.01	114.10
1	A	54	VAL	O-C-N	5.45	129.17	123.02
1	A	104	TRP	CA-C-O	-5.45	112.90	119.49
1	B	118	LYS	N-CA-C	-5.45	106.14	112.89
1	A	49	GLU	CA-C-O	-5.43	114.79	120.55
1	A	106	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	98	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	8	THR	N-CA-C	-5.42	105.92	112.54
1	B	73	THR	CA-C-N	5.42	127.81	120.65
1	B	73	THR	C-N-CA	5.42	127.81	120.65
1	B	45	VAL	N-CA-CB	-5.41	100.28	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	GLU	N-CA-C	-5.41	97.08	107.57
1	B	90	ILE	CA-CB-CG1	5.41	119.59	110.40
1	B	32	GLU	CA-CB-CG	5.39	124.88	114.10
1	A	92	LEU	O-C-N	-5.38	115.44	122.59
1	B	109	SER	CA-CB-OG	5.37	121.84	111.10
1	B	90	ILE	CA-CB-CG2	-5.36	101.39	110.50
1	A	132	ILE	O-C-N	-5.36	115.00	121.10
1	B	73	THR	N-CA-C	-5.35	105.45	111.28
1	A	124	SER	CA-C-O	5.34	125.95	119.11
1	B	17	GLU	CA-CB-CG	5.34	124.78	114.10
1	B	88	ASP	CA-C-O	5.34	126.40	120.63
1	A	7	THR	CB-CA-C	-5.34	100.02	110.11
1	B	122	ASP	CA-C-O	5.33	128.14	120.51
1	A	112	VAL	N-CA-CB	-5.33	101.65	110.56
1	A	130	ASN	CB-CG-ND2	5.33	124.40	116.40
1	B	26	LEU	CD1-CG-CD2	5.33	122.53	110.80
1	B	47	ARG	CA-C-N	5.33	127.74	120.54
1	B	47	ARG	C-N-CA	5.33	127.74	120.54
1	B	78	LYS	O-C-N	5.33	127.77	122.12
1	A	67	THR	O-C-N	-5.32	115.12	122.30
1	A	134	GLY	CA-C-N	5.30	131.66	121.54
1	A	134	GLY	C-N-CA	5.30	131.66	121.54
1	A	15	ILE	CB-CG1-CD1	-5.29	102.70	113.80
1	B	94	ILE	CA-CB-CG1	-5.29	101.41	110.40
1	B	126	SER	N-CA-C	-5.29	102.78	110.08
1	A	81	LEU	N-CA-C	5.29	117.79	111.71
1	A	125	ARG	O-C-N	-5.28	116.83	122.85
1	B	65	THR	N-CA-CB	-5.28	100.98	110.37
1	A	87	THR	N-CA-CB	-5.28	100.03	110.48
1	B	55	VAL	N-CA-CB	-5.26	103.84	111.52
1	B	98	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	124	SER	CB-CA-C	-5.22	100.02	110.42
1	B	123	VAL	CA-C-O	-5.22	114.25	120.78
1	A	50	ARG	NH1-CZ-NH2	-5.22	112.52	119.30
1	B	90	ILE	CG1-CB-CG2	-5.21	95.07	110.70
1	A	108	MET	N-CA-C	5.21	117.53	111.02
1	B	99	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	100	GLU	N-CA-C	-5.20	105.53	111.14
1	B	14	THR	CA-C-O	-5.19	115.05	120.55
1	B	24	THR	CA-C-N	5.19	126.33	119.84
1	B	24	THR	C-N-CA	5.19	126.33	119.84
1	B	104	TRP	CB-CG-CD1	-5.18	119.12	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	THR	CA-C-N	5.18	127.67	120.63
1	A	73	THR	C-N-CA	5.18	127.67	120.63
1	B	9	GLU	CA-CB-CG	-5.17	103.76	114.10
1	A	67	THR	CA-CB-OG1	-5.17	101.85	109.60
1	B	89	ILE	CA-C-O	-5.16	114.33	120.78
1	A	75	VAL	O-C-N	-5.15	116.67	121.87
1	B	96	LYS	CB-CG-CD	5.12	123.08	111.30
1	A	49	GLU	O-C-N	-5.12	116.69	122.12
1	B	29	ARG	N-CA-C	-5.11	104.98	111.11
1	B	130	ASN	N-CA-C	5.11	121.10	109.81
1	A	36	GLN	CA-C-O	-5.10	115.95	121.87
1	A	86	LEU	N-CA-C	5.09	121.65	110.80
1	A	56	VAL	O-C-N	-5.09	117.15	123.10
1	A	70	THR	OG1-CB-CG2	5.09	119.48	109.30
1	B	13	ARG	CA-CB-CG	-5.09	103.93	114.10
1	B	25	PRO	CA-C-O	5.07	129.82	120.60
1	A	87	THR	CA-C-N	5.04	127.00	120.44
1	A	87	THR	C-N-CA	5.04	127.00	120.44
1	B	60	ARG	N-CA-CB	5.01	118.70	110.39
1	A	135	LEU	CA-C-N	5.01	130.71	121.70
1	A	135	LEU	C-N-CA	5.01	130.71	121.70

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 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	1061	0	1080	70	0
1	B	1061	0	1080	69	0
All	All	2122	0	2160	132	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 31.

All (132) 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:108:MET:HE3	1:B:112:VAL:HG12	1.53	0.90
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:108:MET:HE2	1:B:113:GLU:HG3	1.77	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:A:31:ALA:HA	1:A:41:VAL:HG21	1.80	0.62
1:B:23:VAL:HG11	1:B:29:ARG:HH21	1.63	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:A:115:ARG:HH22	1:B:93:ASP:HB2	1.66	0.61
1:B:127:PRO:HG2	1:B:128:PHE:CE1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:SER:OG	1:A:39:PRO:HD2	2.10	0.52
1:A:69:ARG:HG3	1:A:69:ARG:HH11	1.75	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: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:B:88:ASP:CG	1:B:120:LEU:HD21	2.38	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
1:B:108:MET:HE2	1:B:113:GLU:CG	2.42	0.48
1:A:48:MET:HE3	1:A:54:VAL:HG21	1.96	0.48
1:B:83:GLU:HB2	1:B:101:ALA:CB	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:A:69:ARG:HG2	1:A:69:ARG:O	2.13	0.47
1:B:12:LEU:HG	1:B:72:ALA:HB2	1.96	0.47
1:B:24:THR:CB	1:B:60:ARG:HA	2.44	0.47
1:B:21:GLU:CD	1:B:33:ARG:HH21	2.23	0.47
1:B:93:ASP:O	1:B:94:ILE:HB	2.14	0.47
1:B:84:ARG:HH11	1:B:127:PRO:HD3	1.80	0.47
1:B:85:LEU:O	1:B:89:ILE:HB	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:64:MET:HE3	1:A:69:ARG:NH1	2.31	0.45
1:A:17:GLU:HB2	1:A:76:MET:HE1	1.98	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:A:115:ARG:NH2	1:B:93:ASP:HB2	2.31	0.45
1:B:111:GLU:HG3	1:B:114:ARG:HH21	1.81	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:24:THR:HA	1:B:60:ARG:HB3	1.99	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:A:18:LEU:HD23	1:A:33:ARG:NH1	2.32	0.44
1:B:77:ARG:NH1	1:B:134:GLY:HA3	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:B:92:LEU:C	1:B:94:ILE:H	2.26	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:A:84:ARG:HB3	1:A:120:LEU:HD13	2.01	0.43
1:A:77:ARG:NH1	1:A:135:LEU:N	2.64	0.43
1:B:74:ALA:HA	1:B:77:ARG:HD3	1.99	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:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.43
1:B:30:ILE:O	1:B:33:ARG:HB2	2.18	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:11:TYR:OH	1:A:41:VAL:HG22	2.19	0.42
1:A:86:LEU:HB3	1:A:97:VAL:HG22	2.02	0.42
1:A:130:ASN:HA	1:A:131:PRO:HD3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:B:94:ILE:HA	1.97	0.41
1:A:77:ARG:HE	1:A:77:ARG:HB3	1.78	0.41
1:B:128:PHE:CD1	1:B:128:PHE:N	2.88	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 [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	44/226 (20%)	36 (82%)	5 (11%)	3 (7%)	1	5
1	B	121/226 (54%)	90 (74%)	14 (12%)	17 (14%)	0	1
All	All	165/452 (36%)	126 (76%)	19 (12%)	20 (12%)	0	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	B	39	PRO
1	B	59	ASP
1	B	84	ARG
1	B	93	ASP

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Mol	Chain	Res	Type
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	86	LEU
1	B	31	ALA
1	B	70	THR
1	B	134	GLY
1	B	69	ARG
1	B	105	GLU
1	B	61	SER
1	B	123	VAL
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%)	90 (76%)	29 (24%)	1	4
1	B	119/198 (60%)	87 (73%)	32 (27%)	0	2
All	All	238/396 (60%)	177 (74%)	61 (26%)	0	3

All (61) 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

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Mol	Chain	Res	Type
1	A	44	THR
1	A	51	ASP
1	A	54	VAL
1	A	59	ASP
1	A	60	ARG
1	A	62	LEU
1	A	77	ARG
1	A	88	ASP
1	A	89	ILE
1	A	95	ASN
1	A	96	LYS
1	A	97	VAL
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	123	VAL
1	A	125	ARG
1	A	132	ILE
1	B	6	ASP
1	B	10	MET
1	B	13	ARG
1	B	26	LEU
1	B	29	ARG
1	B	30	ILE
1	B	32	GLU
1	B	35	GLU
1	B	39	PRO
1	B	40	THR
1	B	44	THR
1	B	48	MET
1	B	51	ASP
1	B	67	THR
1	B	77	ARG
1	B	81	LEU
1	B	83	GLU
1	B	84	ARG
1	B	85	LEU
1	B	87	THR
1	B	90	ILE

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Mol	Chain	Res	Type
1	B	92	LEU
1	B	94	ILE
1	B	100	GLU
1	B	117	VAL
1	B	120	LEU
1	B	124	SER
1	B	125	ARG
1	B	130	ASN
1	B	133	PRO
1	B	135	LEU
1	B	136	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.