



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:54 PM UTC

PDB ID : 1CTX / pdb_00001ctx
Title : THREE-DIMENSIONAL STRUCTURE OF THE-LONG-NEUROTOXIN
FROM COBRA VENOM
Authors : Saenger, W.; Walkinshaw, M.D.
Deposited on : 1982-04-08
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

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

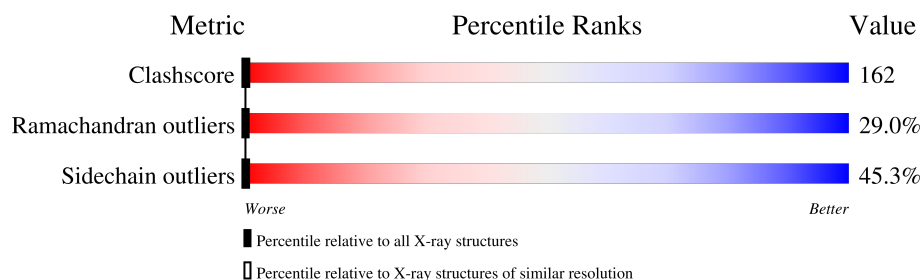
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

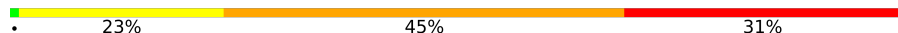
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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	71	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 541 atoms, of which 0 are hydrogens and 0 are deuteriums.

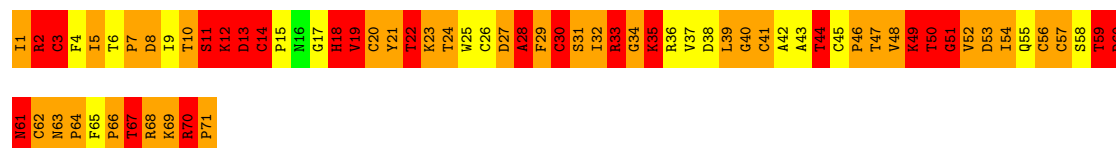
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA-COBRATOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	71	541	332	98	101	10	0	0	0

Note EDS was not executed.

Chain A: 23% 45% 31%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.60Å 74.60Å 42.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	541	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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	3.99	56/553 (10.1%)	2.71	33/750 (4.4%)

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	1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	C-OXT	44.46	2.12	1.23
1	A	14	CYS	CA-CB	-30.35	1.05	1.53
1	A	3	CYS	N-CA	26.92	1.79	1.46
1	A	14	CYS	CB-SG	18.06	2.40	1.81
1	A	3	CYS	CA-C	15.93	1.72	1.52
1	A	51	GLY	N-CA	9.91	1.59	1.45
1	A	19	VAL	CA-CB	-9.90	1.41	1.54
1	A	38	ASP	CA-C	9.14	1.63	1.52
1	A	40	GLY	N-CA	9.10	1.55	1.45
1	A	10	THR	N-CA	8.85	1.56	1.45
1	A	70	ARG	N-CA	8.68	1.58	1.46
1	A	49	LYS	CA-C	8.29	1.63	1.52
1	A	36	ARG	NE-CZ	8.11	1.42	1.33
1	A	23	LYS	N-CA	8.04	1.55	1.45
1	A	22	THR	CA-C	8.01	1.62	1.52
1	A	27	ASP	CA-C	7.95	1.62	1.52
1	A	18	HIS	CE1-NE2	-7.94	1.24	1.32
1	A	40	GLY	CA-C	7.33	1.59	1.51
1	A	33	ARG	CA-C	7.29	1.60	1.52
1	A	13	ASP	N-CA	7.27	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	CA-C	-7.25	1.37	1.52
1	A	51	GLY	CA-C	7.23	1.62	1.51
1	A	71	PRO	N-CA	7.12	1.57	1.47
1	A	44	THR	CA-CB	6.99	1.65	1.53
1	A	29	PHE	CA-C	6.94	1.62	1.52
1	A	34	GLY	N-CA	6.94	1.51	1.45
1	A	26	CYS	N-CA	6.91	1.54	1.45
1	A	50	THR	CA-C	6.88	1.61	1.52
1	A	70	ARG	CD-NE	6.64	1.55	1.46
1	A	58	SER	N-CA	-6.53	1.38	1.46
1	A	60	ASP	CG-OD1	6.50	1.37	1.25
1	A	12	LYS	CA-C	6.49	1.61	1.52
1	A	25	TRP	NE1-CE2	-6.30	1.30	1.37
1	A	18	HIS	CB-CG	6.12	1.58	1.50
1	A	33	ARG	N-CA	-6.12	1.39	1.46
1	A	12	LYS	N-CA	6.12	1.54	1.46
1	A	65	PHE	CA-C	6.11	1.60	1.52
1	A	69	LYS	N-CA	6.05	1.54	1.46
1	A	28	ALA	N-CA	6.00	1.53	1.46
1	A	66	PRO	CA-CB	-5.91	1.45	1.53
1	A	25	TRP	N-CA	5.73	1.53	1.45
1	A	25	TRP	CA-C	5.69	1.59	1.52
1	A	14	CYS	CA-C	-5.65	1.45	1.52
1	A	45	CYS	CA-C	5.64	1.60	1.52
1	A	57	CYS	CA-C	5.59	1.59	1.52
1	A	52	VAL	N-CA	5.58	1.52	1.46
1	A	18	HIS	N-CA	5.53	1.54	1.46
1	A	46	PRO	C-O	5.52	1.30	1.23
1	A	18	HIS	CG-CD2	-5.41	1.29	1.35
1	A	35	LYS	C-O	5.34	1.31	1.23
1	A	47	THR	C-O	5.30	1.30	1.23
1	A	33	ARG	NE-CZ	-5.28	1.27	1.33
1	A	66	PRO	N-CA	5.12	1.53	1.47
1	A	68	ARG	CA-C	5.11	1.59	1.52
1	A	18	HIS	CA-C	5.06	1.59	1.53
1	A	59	THR	C-O	5.06	1.30	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CYS	CB-CA-C	30.30	147.07	109.80
1	A	49	LYS	O-C-N	13.12	140.04	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CYS	N-CA-C	-12.85	91.62	110.64
1	A	3	CYS	CA-C-O	-12.11	109.50	120.88
1	A	2	ARG	CA-C-N	12.00	142.73	121.97
1	A	2	ARG	C-N-CA	12.00	142.73	121.97
1	A	14	CYS	N-CA-CB	-11.74	89.47	110.37
1	A	49	LYS	CA-C-N	10.65	141.89	121.54
1	A	49	LYS	C-N-CA	10.65	141.89	121.54
1	A	62	CYS	N-CA-C	7.93	121.95	107.99
1	A	7	PRO	O-C-N	7.68	135.69	121.10
1	A	14	CYS	N-CA-C	7.50	126.40	109.81
1	A	40	GLY	O-C-N	6.86	131.40	123.51
1	A	57	CYS	O-C-N	6.71	130.91	123.33
1	A	19	VAL	O-C-N	6.67	130.91	122.57
1	A	70	ARG	N-CA-C	-6.67	95.06	109.81
1	A	52	VAL	CB-CA-C	-6.65	102.02	111.40
1	A	33	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	62	CYS	CB-CA-C	-6.43	100.36	111.30
1	A	3	CYS	N-CA-CB	6.19	118.72	109.19
1	A	20	CYS	O-C-N	6.18	131.18	123.14
1	A	70	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	A	14	CYS	O-C-N	-5.80	114.65	121.32
1	A	61	ASN	CB-CA-C	-5.77	98.93	110.42
1	A	58	SER	O-C-N	5.72	128.21	122.03
1	A	46	PRO	O-C-N	5.67	129.77	122.91
1	A	10	THR	CB-CA-C	5.53	120.22	109.33
1	A	56	CYS	O-C-N	5.53	129.57	123.33
1	A	14	CYS	CB-CA-C	5.33	120.66	110.17
1	A	45	CYS	CA-C-O	5.25	124.65	119.51
1	A	38	ASP	O-C-N	5.07	129.54	123.36
1	A	60	ASP	O-C-N	5.03	129.28	122.59
1	A	45	CYS	O-C-N	-5.02	116.94	121.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	CYS	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	541	0	524	173	10
All	All	541	0	524	173	10

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 162.

All (173) 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:A:1:ILE:CD1	1:A:19:VAL:N	1.69	1.52
1:A:3:CYS:CA	1:A:3:CYS:N	1.79	1.46
1:A:50:THR:CG2	1:A:51:GLY:H	1.54	1.19
1:A:4:PHE:HB2	1:A:63:ASN:HB3	1.27	1.15
1:A:63:ASN:H	1:A:64:PRO:HD3	1.02	1.14
1:A:2:ARG:HD3	1:A:12:LYS:HB3	1.32	1.12
1:A:23:LYS:HB3	1:A:54:ILE:HB	1.28	1.11
1:A:2:ARG:HD3	1:A:12:LYS:CB	1.81	1.10
1:A:14:CYS:CB	1:A:14:CYS:SG	2.40	1.09
1:A:67:THR:OG1	1:A:71:PRO:C	1.95	1.09
1:A:1:ILE:HD12	1:A:19:VAL:N	1.43	1.08
1:A:50:THR:HG22	1:A:51:GLY:H	1.08	1.08
1:A:1:ILE:HD13	1:A:19:VAL:N	1.61	1.07
1:A:67:THR:O	1:A:69:LYS:N	1.86	1.07
1:A:2:ARG:O	1:A:12:LYS:HG2	1.56	1.06
1:A:3:CYS:HB2	1:A:41:CYS:HB2	1.08	1.06
1:A:2:ARG:HB2	1:A:60:ASP:HB3	1.33	1.04
1:A:3:CYS:CB	1:A:41:CYS:HB2	1.87	1.02
1:A:1:ILE:HD11	1:A:3:CYS:SG	2.00	1.00
1:A:33:ARG:O	1:A:33:ARG:HG3	1.61	0.98
1:A:63:ASN:N	1:A:64:PRO:HD3	1.77	0.98
1:A:63:ASN:H	1:A:64:PRO:CD	1.75	0.98
1:A:67:THR:OG1	1:A:71:PRO:O	1.84	0.96
1:A:1:ILE:HD11	1:A:19:VAL:O	1.66	0.95
1:A:53:ASP:OD1	1:A:70:ARG:HD2	1.66	0.95
1:A:12:LYS:HE2	1:A:61:ASN:HA	1.48	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:THR:CG2	1:A:39:LEU:H	1.81	0.94
1:A:48:VAL:HG22	1:A:49:LYS:N	1.84	0.93
1:A:50:THR:CG2	1:A:51:GLY:N	2.25	0.93
1:A:2:ARG:CD	1:A:12:LYS:HB3	2.00	0.92
1:A:48:VAL:HG22	1:A:49:LYS:H	1.33	0.92
1:A:50:THR:HG22	1:A:51:GLY:N	1.81	0.91
1:A:71:PRO:C	1:A:71:PRO:OXT	2.12	0.91
1:A:59:THR:HB	1:A:62:CYS:SG	2.12	0.90
1:A:1:ILE:CD1	1:A:19:VAL:CA	2.51	0.89
1:A:43:ALA:O	1:A:44:THR:HB	1.71	0.88
1:A:1:ILE:HD11	1:A:19:VAL:C	1.99	0.87
1:A:1:ILE:HD11	1:A:19:VAL:N	1.90	0.87
1:A:63:ASN:N	1:A:64:PRO:CD	2.33	0.86
1:A:19:VAL:HG13	1:A:20:CYS:N	1.91	0.85
1:A:24:THR:OG1	1:A:35:LYS:HD3	1.77	0.85
1:A:1:ILE:HG21	1:A:18:HIS:HA	1.58	0.84
1:A:3:CYS:HB2	1:A:41:CYS:CB	2.01	0.84
1:A:21:TYR:CD2	1:A:21:TYR:O	2.30	0.84
1:A:2:ARG:NH1	1:A:12:LYS:HB2	1.94	0.83
1:A:11:SER:O	1:A:12:LYS:HG3	1.81	0.80
1:A:2:ARG:HH11	1:A:12:LYS:HB2	1.45	0.80
1:A:21:TYR:CD2	1:A:21:TYR:C	2.59	0.80
1:A:71:PRO:O	1:A:71:PRO:OXT	1.97	0.80
1:A:6:THR:HG21	1:A:39:LEU:H	1.45	0.79
1:A:1:ILE:HD12	1:A:19:VAL:CA	2.12	0.79
1:A:11:SER:O	1:A:12:LYS:CG	2.30	0.79
1:A:6:THR:CG2	1:A:39:LEU:HB2	2.13	0.78
1:A:70:ARG:HA	1:A:71:PRO:OXT	1.82	0.78
1:A:50:THR:HG23	1:A:51:GLY:H	1.48	0.78
1:A:6:THR:HB	1:A:7:PRO:HA	1.67	0.76
1:A:35:LYS:NZ	1:A:69:LYS:O	2.18	0.76
1:A:39:LEU:HG	1:A:63:ASN:O	1.86	0.75
1:A:1:ILE:HG23	1:A:15:PRO:O	1.86	0.75
1:A:4:PHE:HB2	1:A:63:ASN:CB	2.14	0.75
1:A:53:ASP:CG	1:A:70:ARG:HD2	2.13	0.74
1:A:12:LYS:CE	1:A:61:ASN:HA	2.17	0.74
1:A:48:VAL:CG2	1:A:49:LYS:N	2.50	0.74
1:A:24:THR:OG1	1:A:35:LYS:CD	2.35	0.74
1:A:6:THR:HG23	1:A:39:LEU:HB2	1.68	0.73
1:A:13:ASP:O	1:A:14:CYS:CB	2.33	0.73
1:A:6:THR:HG23	1:A:39:LEU:H	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:O	1:A:29:PHE:N	2.22	0.73
1:A:41:CYS:SG	1:A:41:CYS:O	2.46	0.73
1:A:2:ARG:HB3	1:A:12:LYS:HG2	1.70	0.72
1:A:54:ILE:HG13	1:A:55:GLN:N	2.05	0.71
1:A:30:CYS:HA	1:A:34:GLY:O	1.90	0.71
1:A:17:GLY:HA2	1:A:43:ALA:HB2	1.72	0.70
1:A:23:LYS:HB3	1:A:54:ILE:CB	2.16	0.70
1:A:57:CYS:SG	1:A:62:CYS:O	2.50	0.69
1:A:1:ILE:HD11	1:A:19:VAL:CA	2.21	0.68
1:A:3:CYS:N	1:A:3:CYS:C	2.52	0.68
1:A:17:GLY:C	1:A:18:HIS:CD2	2.72	0.68
1:A:59:THR:O	1:A:62:CYS:SG	2.53	0.66
1:A:67:THR:C	1:A:69:LYS:H	1.99	0.66
1:A:13:ASP:O	1:A:14:CYS:HB3	1.73	0.66
1:A:50:THR:HG23	1:A:51:GLY:N	2.09	0.66
1:A:5:ILE:N	1:A:63:ASN:OD1	2.25	0.66
1:A:4:PHE:HE2	1:A:10:THR:HB	1.61	0.65
1:A:17:GLY:C	1:A:18:HIS:CG	2.75	0.65
1:A:19:VAL:HG22	1:A:57:CYS:O	1.97	0.64
1:A:4:PHE:CE2	1:A:10:THR:HB	2.32	0.64
1:A:4:PHE:CD2	1:A:10:THR:HA	2.33	0.64
1:A:3:CYS:CB	1:A:41:CYS:CB	2.68	0.63
1:A:6:THR:HG23	1:A:39:LEU:N	2.13	0.63
1:A:70:ARG:CA	1:A:71:PRO:C	2.71	0.63
1:A:53:ASP:CG	1:A:70:ARG:CD	2.72	0.63
1:A:70:ARG:HA	1:A:71:PRO:C	2.23	0.63
1:A:1:ILE:HG21	1:A:18:HIS:CA	2.29	0.62
1:A:6:THR:HG23	1:A:39:LEU:CB	2.29	0.62
1:A:2:ARG:HD3	1:A:12:LYS:HB2	1.78	0.62
1:A:70:ARG:CA	1:A:71:PRO:OXT	2.48	0.62
1:A:2:ARG:HB3	1:A:12:LYS:CG	2.30	0.61
1:A:17:GLY:HA3	1:A:42:ALA:O	1.98	0.61
1:A:64:PRO:O	1:A:66:PRO:HD3	2.00	0.61
1:A:6:THR:CG2	1:A:39:LEU:N	2.60	0.60
1:A:6:THR:HG23	1:A:39:LEU:CA	2.31	0.60
1:A:6:THR:N	1:A:39:LEU:O	2.35	0.60
1:A:4:PHE:CE1	1:A:61:ASN:O	2.55	0.59
1:A:59:THR:O	1:A:60:ASP:C	2.45	0.59
1:A:69:LYS:O	1:A:70:ARG:HB3	2.01	0.59
1:A:39:LEU:HG	1:A:63:ASN:ND2	2.18	0.58
1:A:1:ILE:HD12	1:A:18:HIS:C	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:CG	1:A:70:ARG:NE	2.61	0.58
1:A:30:CYS:SG	1:A:35:LYS:HA	2.44	0.58
1:A:66:PRO:O	1:A:67:THR:C	2.48	0.56
1:A:21:TYR:CD1	1:A:46:PRO:HG3	2.40	0.56
1:A:14:CYS:SG	1:A:14:CYS:CA	2.91	0.55
1:A:23:LYS:CB	1:A:54:ILE:HB	2.20	0.55
1:A:2:ARG:CD	1:A:12:LYS:CB	2.68	0.55
1:A:1:ILE:CD1	1:A:18:HIS:C	2.71	0.55
1:A:6:THR:HG22	1:A:39:LEU:HB2	1.88	0.54
1:A:11:SER:O	1:A:12:LYS:HD2	2.08	0.54
1:A:53:ASP:OD1	1:A:53:ASP:C	2.50	0.54
1:A:66:PRO:HB2	1:A:71:PRO:OXT	2.09	0.52
1:A:48:VAL:O	1:A:49:LYS:O	2.28	0.52
1:A:5:ILE:HA	1:A:40:GLY:HA2	1.92	0.52
1:A:18:HIS:O	1:A:19:VAL:HB	2.11	0.51
1:A:63:ASN:O	1:A:63:ASN:CG	2.53	0.51
1:A:17:GLY:CA	1:A:43:ALA:HB2	2.40	0.51
1:A:30:CYS:O	1:A:31:SER:C	2.54	0.51
1:A:11:SER:O	1:A:12:LYS:CD	2.59	0.50
1:A:6:THR:HG23	1:A:39:LEU:O	2.10	0.50
1:A:67:THR:C	1:A:69:LYS:N	2.64	0.49
1:A:30:CYS:SG	1:A:35:LYS:CG	3.00	0.49
1:A:32:ILE:HD13	1:A:33:ARG:N	2.28	0.49
1:A:2:ARG:CB	1:A:12:LYS:HB3	2.43	0.48
1:A:21:TYR:C	1:A:21:TYR:HD2	2.17	0.48
1:A:1:ILE:CD1	1:A:3:CYS:SG	2.88	0.48
1:A:4:PHE:HD2	1:A:11:SER:H	1.61	0.48
1:A:1:ILE:CG2	1:A:15:PRO:O	2.60	0.47
1:A:2:ARG:CG	1:A:12:LYS:HB3	2.45	0.47
1:A:17:GLY:CA	1:A:42:ALA:O	2.63	0.46
1:A:21:TYR:CE2	1:A:23:LYS:HE2	2.50	0.46
1:A:39:LEU:CG	1:A:63:ASN:O	2.62	0.46
1:A:21:TYR:O	1:A:21:TYR:CG	2.69	0.46
1:A:2:ARG:O	1:A:60:ASP:O	2.34	0.45
1:A:30:CYS:SG	1:A:35:LYS:HG2	2.57	0.45
1:A:62:CYS:SG	1:A:62:CYS:O	2.75	0.44
1:A:22:THR:HG22	1:A:63:ASN:HD22	1.82	0.44
1:A:3:CYS:O	1:A:12:LYS:HA	2.18	0.44
1:A:4:PHE:HD2	1:A:10:THR:HA	1.82	0.44
1:A:30:CYS:SG	1:A:35:LYS:HG3	2.57	0.43
1:A:2:ARG:HA	1:A:13:ASP:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:O	1:A:30:CYS:O	2.36	0.43
1:A:3:CYS:HB3	1:A:41:CYS:CB	2.49	0.43
1:A:49:LYS:HA	1:A:49:LYS:HD3	1.61	0.43
1:A:24:THR:OG1	1:A:35:LYS:HD2	2.17	0.43
1:A:44:THR:O	1:A:46:PRO:HD3	2.19	0.43
1:A:5:ILE:HG12	1:A:41:CYS:HB3	2.00	0.43
1:A:12:LYS:HB3	1:A:13:ASP:H	1.64	0.43
1:A:5:ILE:CG1	1:A:41:CYS:HB3	2.49	0.42
1:A:1:ILE:CG2	1:A:18:HIS:HA	2.39	0.42
1:A:33:ARG:O	1:A:33:ARG:CG	2.44	0.42
1:A:53:ASP:OD1	1:A:70:ARG:CD	2.51	0.42
1:A:11:SER:O	1:A:12:LYS:CB	2.67	0.42
1:A:30:CYS:HB3	1:A:31:SER:H	1.48	0.42
1:A:53:ASP:CB	1:A:70:ARG:CZ	2.98	0.42
1:A:27:ASP:O	1:A:28:ALA:C	2.62	0.42
1:A:67:THR:CB	1:A:71:PRO:C	2.88	0.41
1:A:19:VAL:HG22	1:A:20:CYS:H	1.86	0.41
1:A:29:PHE:O	1:A:32:ILE:HD13	2.19	0.41
1:A:32:ILE:CD1	1:A:32:ILE:N	2.84	0.41
1:A:2:ARG:HE	1:A:13:ASP:HB2	1.86	0.41
1:A:7:PRO:CD	1:A:8:ASP:H	2.32	0.41
1:A:29:PHE:O	1:A:30:CYS:C	2.64	0.41
1:A:52:VAL:HG12	1:A:53:ASP:N	2.35	0.40
1:A:30:CYS:O	1:A:34:GLY:N	2.50	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:CG2	1:A:28:ALA:N[5_565]	0.54	1.66
1:A:53:ASP:OD1	1:A:55:GLN:OE1[7_555]	1.30	0.90
1:A:71:PRO:O	1:A:71:PRO:O[7_555]	1.43	0.77
1:A:10:THR:CG2	1:A:27:ASP:C[5_565]	1.46	0.74
1:A:54:ILE:O	1:A:55:GLN:CG[7_555]	1.51	0.69
1:A:10:THR:CG2	1:A:28:ALA:CA[5_565]	1.55	0.65
1:A:14:CYS:O	1:A:14:CYS:O[10_665]	1.62	0.58
1:A:10:THR:CB	1:A:28:ALA:N[5_565]	1.76	0.44
1:A:53:ASP:CG	1:A:55:GLN:OE1[7_555]	1.94	0.26
1:A:67:THR:OG1	1:A:71:PRO:CB[7_555]	2.11	0.09

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	69/71 (97%)	33 (48%)	16 (23%)	20 (29%)	0 0

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	ASP
1	A	12	LYS
1	A	13	ASP
1	A	28	ALA
1	A	30	CYS
1	A	31	SER
1	A	44	THR
1	A	49	LYS
1	A	63	ASN
1	A	68	ARG
1	A	11	SER
1	A	19	VAL
1	A	51	GLY
1	A	59	THR
1	A	60	ASP
1	A	67	THR
1	A	9	ILE
1	A	64	PRO
1	A	70	ARG

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	64/64 (100%)	35 (55%)	29 (45%)	0 0

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	2	ARG
1	A	11	SER
1	A	14	CYS
1	A	18	HIS
1	A	19	VAL
1	A	21	TYR
1	A	22	THR
1	A	24	THR
1	A	30	CYS
1	A	32	ILE
1	A	33	ARG
1	A	35	LYS
1	A	37	VAL
1	A	39	LEU
1	A	41	CYS
1	A	44	THR
1	A	47	THR
1	A	48	VAL
1	A	49	LYS
1	A	50	THR
1	A	53	ASP
1	A	54	ILE
1	A	56	CYS
1	A	59	THR
1	A	60	ASP
1	A	61	ASN
1	A	67	THR
1	A	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	55	GLN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.