



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:48 AM UTC

PDB ID : 1RH1 / pdb_00001rh1
Title : crystal structure of the cytotoxic bacterial protein colicin B at 2.5 Å resolution
Authors : Hilsenbeck, J.L.; Park, H.; Chen, G.; Youn, B.; Postle, K.; Kang, C.
Deposited on : 2003-11-13
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

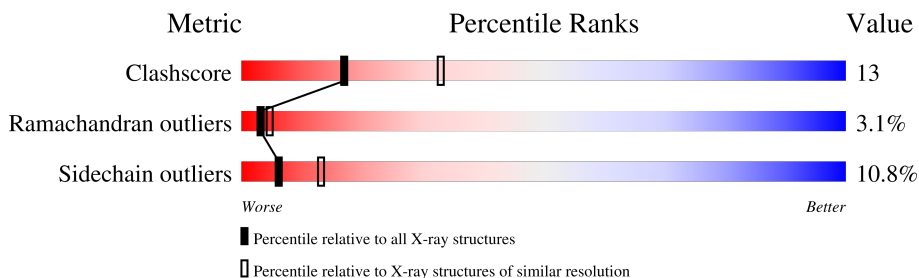
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	511	59% 28% 6% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3902 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 Colicin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3718	2346	630	729	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P05819

- Molecule 2 is water.

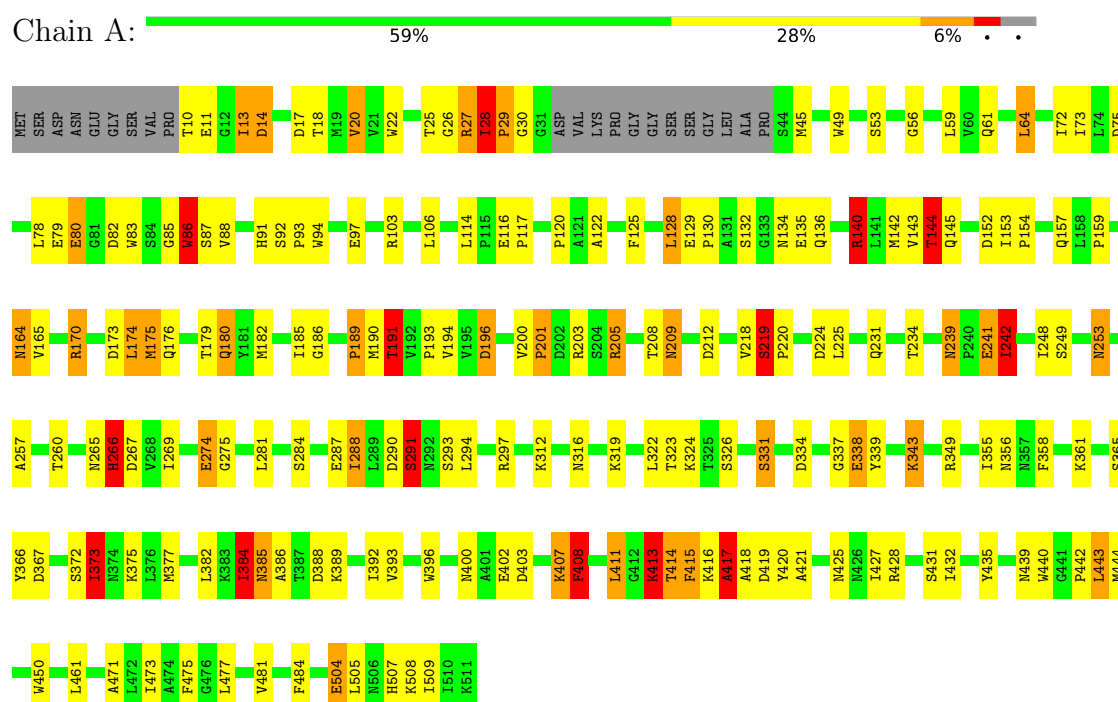
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total	O	0	0
			184	184		

3 Residue-property plots

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: Colicin B



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.16 Å 138.17 Å 106.16 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3902	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.96	3/3789 (0.1%)	1.87	96/5149 (1.9%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	507	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	266	HIS	CD2-NE2	-5.45	1.31	1.37

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ASP	CA-CB-CG	10.14	122.74	112.60
1	A	80	GLU	CB-CG-CD	9.55	128.84	112.60
1	A	173	ASP	CA-CB-CG	9.51	122.11	112.60
1	A	415	PHE	CA-CB-CG	9.09	122.89	113.80
1	A	338	GLU	CB-CG-CD	8.38	126.86	112.60
1	A	241	GLU	N-CA-C	8.19	120.12	111.03
1	A	407	LYS	CA-C-N	8.11	137.04	121.54
1	A	407	LYS	C-N-CA	8.11	137.04	121.54
1	A	82	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	209	ASN	CA-CB-CG	7.63	120.23	112.60
1	A	415	PHE	CA-C-N	7.58	136.03	121.54
1	A	415	PHE	C-N-CA	7.58	136.03	121.54
1	A	128	LEU	N-CA-C	7.50	120.75	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MET	CG-SD-CE	-7.48	84.44	100.90
1	A	267	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	29	PRO	N-CA-C	7.33	127.57	112.47
1	A	196	ASP	N-CA-C	7.31	120.43	108.52
1	A	418	ALA	N-CA-C	7.13	120.72	109.39
1	A	253	ASN	N-CA-C	7.04	125.81	110.80
1	A	418	ALA	CA-C-N	7.02	133.42	122.26
1	A	418	ALA	C-N-CA	7.02	133.42	122.26
1	A	125	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	291	SER	N-CA-C	6.82	125.32	110.80
1	A	144	THR	CA-CB-OG1	-6.78	99.42	109.60
1	A	53	SER	CA-C-N	6.72	126.86	119.87
1	A	53	SER	C-N-CA	6.72	126.86	119.87
1	A	49	TRP	N-CA-C	6.68	119.39	111.71
1	A	384	ILE	CB-CA-C	-6.67	100.69	110.62
1	A	413	LYS	CA-C-O	6.65	126.22	119.97
1	A	414	THR	N-CA-C	6.51	119.43	108.23
1	A	14	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	509	ILE	N-CA-C	6.45	117.10	111.56
1	A	80	GLU	N-CA-C	-6.41	105.44	113.20
1	A	28	ILE	CA-C-N	6.36	127.79	119.84
1	A	28	ILE	C-N-CA	6.36	127.79	119.84
1	A	414	THR	CA-C-N	6.33	133.63	121.54
1	A	414	THR	C-N-CA	6.33	133.63	121.54
1	A	367	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	407	LYS	O-C-N	6.19	130.90	122.48
1	A	290	ASP	CA-CB-CG	6.17	118.78	112.60
1	A	435	TYR	N-CA-C	-6.12	104.16	111.69
1	A	191	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	334	ASP	CA-C-O	-6.05	114.64	121.00
1	A	86	TRP	N-CA-C	6.03	119.22	109.40
1	A	414	THR	CA-C-O	-5.90	114.61	120.98
1	A	417	ALA	N-CA-C	5.79	123.14	110.80
1	A	144	THR	CA-CB-CG2	5.78	120.32	110.50
1	A	170	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	507	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	A	22	TRP	N-CA-C	-5.70	100.38	109.04
1	A	152	ASP	N-CA-C	5.70	120.22	113.16
1	A	193	PRO	N-CA-C	5.63	119.70	111.03
1	A	471	ALA	N-CA-C	-5.60	104.67	112.45
1	A	200	VAL	CA-C-N	5.60	125.52	119.76
1	A	200	VAL	C-N-CA	5.60	125.52	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ASP	N-CA-C	-5.57	106.48	113.72
1	A	365	SER	CA-C-N	5.55	128.03	120.54
1	A	365	SER	C-N-CA	5.55	128.03	120.54
1	A	218	VAL	N-CA-C	-5.53	105.13	110.72
1	A	421	ALA	CA-C-N	5.49	127.48	120.56
1	A	421	ALA	C-N-CA	5.49	127.48	120.56
1	A	80	GLU	CB-CA-C	5.48	120.52	110.11
1	A	418	ALA	CA-C-O	5.46	129.47	122.64
1	A	201	PRO	N-CA-C	5.43	119.61	111.14
1	A	180	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	205	ARG	CA-C-N	5.42	125.36	119.78
1	A	205	ARG	C-N-CA	5.42	125.36	119.78
1	A	85	GLY	O-C-N	5.40	129.72	122.70
1	A	13	ILE	CA-C-N	5.35	127.71	120.38
1	A	13	ILE	C-N-CA	5.35	127.71	120.38
1	A	83	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	A	140	ARG	CA-CB-CG	-5.33	103.43	114.10
1	A	164	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	396	TRP	CE2-CD2-CG	-5.29	100.86	107.20
1	A	407	LYS	N-CA-C	5.20	116.96	108.63
1	A	136	GLN	CB-CG-CD	5.18	121.40	112.60
1	A	91	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	A	224	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	86	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	440	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	431	SER	N-CA-C	-5.15	105.74	112.23
1	A	26	GLY	CA-C-N	5.15	131.37	121.54
1	A	26	GLY	C-N-CA	5.15	131.37	121.54
1	A	408	PHE	N-CA-CB	5.14	119.18	110.49
1	A	28	ILE	CA-CB-CG2	-5.13	101.79	110.50
1	A	144	THR	N-CA-CB	-5.07	102.14	111.37
1	A	191	THR	CA-CB-CG2	5.06	119.11	110.50
1	A	212	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	17	ASP	CA-C-N	5.06	131.21	123.47
1	A	17	ASP	C-N-CA	5.06	131.21	123.47
1	A	373	ILE	CB-CG1-CD1	-5.05	103.19	113.80
1	A	316	ASN	N-CA-C	-5.05	105.42	111.03
1	A	114	LEU	CA-C-N	5.03	124.47	119.24
1	A	114	LEU	C-N-CA	5.03	124.47	119.24
1	A	22	TRP	CE2-CD2-CG	-5.01	101.18	107.20
1	A	440	TRP	CG-CD2-CE3	5.01	138.91	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	SER	Peptide
1	A	28	ILE	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	3718	0	3701	94	0
2	A	184	0	0	3	0
All	All	3902	0	3701	94	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 13.

All (94) 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:265:ASN:HD21	1:A:287:GLU:H	1.22	0.86
1:A:324:LYS:HE3	1:A:411:LEU:HG	1.67	0.76
1:A:385:ASN:H	1:A:385:ASN:HD22	1.40	0.70
1:A:265:ASN:ND2	1:A:287:GLU:H	1.90	0.69
1:A:56:GLY:HA3	1:A:203:ARG:HE	1.60	0.64
1:A:274:GLU:HG3	1:A:275:GLY:H	1.63	0.64
1:A:475:PHE:HB3	1:A:477:LEU:HG	1.81	0.63
1:A:373:ILE:HG21	1:A:444:MET:HE2	1.81	0.63
1:A:10:THR:HG22	1:A:11:GLU:H	1.63	0.62
1:A:103:ARG:HH12	1:A:145:GLN:HE22	1.48	0.61
1:A:407:LYS:HB3	1:A:411:LEU:HD22	1.82	0.61
1:A:384:ILE:HD12	1:A:484:PHE:CZ	2.34	0.61
1:A:130:PRO:HB3	1:A:294:LEU:HD11	1.83	0.60
1:A:14:ASP:HB2	1:A:191:THR:HG22	1.84	0.60
1:A:343:LYS:HE2	1:A:508:LYS:HB3	1.84	0.60
1:A:94:TRP:HZ3	1:A:242:ILE:HD11	1.67	0.59
1:A:425:ASN:HD22	1:A:428:ARG:HH21	1.50	0.58
1:A:219:SER:OG	1:A:220:PRO:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PHE:HD1	1:A:414:THR:O	1.87	0.56
1:A:408:PHE:HA	1:A:414:THR:H	1.71	0.56
1:A:20:VAL:O	1:A:260:THR:HA	2.06	0.55
1:A:29:PRO:HA	1:A:135:GLU:O	2.07	0.55
1:A:439:ASN:OD1	1:A:442:PRO:HD2	2.06	0.55
1:A:59:LEU:O	1:A:87:SER:HB2	2.08	0.54
1:A:174:LEU:HD13	1:A:176:GLN:HG3	1.88	0.54
1:A:142:MET:HA	1:A:284:SER:O	2.08	0.53
1:A:159:PRO:HD2	1:A:194:VAL:HG21	1.90	0.53
1:A:477:LEU:HD13	1:A:481:VAL:HG12	1.89	0.53
1:A:175:MET:SD	1:A:297:ARG:HD3	2.49	0.53
1:A:120:PRO:HG2	1:A:257:ALA:HB3	1.91	0.52
1:A:400:ASN:ND2	1:A:403:ASP:H	2.07	0.52
1:A:180:GLN:HE22	1:A:288:ILE:HA	1.73	0.52
1:A:393:VAL:HG13	1:A:432:ILE:HG23	1.91	0.51
1:A:408:PHE:HA	1:A:414:THR:N	2.25	0.51
1:A:28:ILE:H	1:A:28:ILE:HD13	1.75	0.51
1:A:291:SER:HA	1:A:294:LEU:HD12	1.93	0.51
1:A:504:GLU:HG3	1:A:508:LYS:HE2	1.92	0.51
1:A:384:ILE:HG12	1:A:389:LYS:HE3	1.93	0.50
1:A:400:ASN:HD21	1:A:402:GLU:HB2	1.77	0.50
1:A:201:PRO:HA	1:A:209:ASN:HA	1.93	0.49
1:A:27:ARG:HB2	2:A:2153:HOH:O	2.12	0.49
1:A:427:ILE:HD11	1:A:450:TRP:CH2	2.48	0.49
1:A:186:GLY:HA2	1:A:190:MET:CE	2.43	0.48
1:A:165:VAL:HG11	1:A:269:ILE:HD12	1.96	0.48
1:A:25:THR:HB	1:A:293:SER:OG	2.13	0.48
1:A:288:ILE:HD12	1:A:288:ILE:H	1.79	0.48
1:A:319:LYS:O	1:A:323:THR:HG23	2.13	0.48
1:A:128:LEU:HD23	1:A:180:GLN:HE21	1.79	0.48
1:A:358:PHE:HA	1:A:361:LYS:HD2	1.95	0.47
1:A:408:PHE:O	1:A:413:LYS:HA	2.13	0.47
1:A:220:PRO:HD3	1:A:266:HIS:HB2	1.96	0.47
1:A:372:SER:O	1:A:375:LYS:HB3	2.15	0.47
1:A:88:VAL:HG13	1:A:225:LEU:HD11	1.97	0.47
1:A:64:LEU:HD22	1:A:88:VAL:HG21	1.97	0.46
1:A:326:SER:HB2	1:A:356:ASN:HD22	1.81	0.46
1:A:417:ALA:O	1:A:420:TYR:HD1	1.99	0.46
1:A:239:ASN:HD22	1:A:241:GLU:H	1.62	0.46
1:A:128:LEU:HD23	1:A:180:GLN:NE2	2.31	0.46
1:A:116:GLU:HA	1:A:117:PRO:HD2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD22	1:A:355:ILE:O	2.16	0.46
1:A:174:LEU:HD22	2:A:1367:HOH:O	2.15	0.45
1:A:186:GLY:HA2	1:A:190:MET:HE1	1.97	0.45
1:A:154:PRO:HD2	1:A:157:GLN:HB2	1.97	0.45
1:A:75:ASP:HB3	1:A:78:LEU:HB2	1.99	0.45
1:A:274:GLU:HG3	1:A:275:GLY:N	2.28	0.45
1:A:323:THR:HA	1:A:356:ASN:HD21	1.80	0.45
1:A:11:GLU:O	1:A:14:ASP:HB3	2.17	0.44
1:A:219:SER:CB	1:A:220:PRO:HA	2.47	0.44
1:A:385:ASN:H	1:A:385:ASN:ND2	2.10	0.44
1:A:231:GLN:HB2	1:A:234:THR:HG23	2.00	0.44
1:A:425:ASN:ND2	1:A:428:ARG:HH21	2.15	0.44
1:A:337:GLY:C	1:A:339:TYR:H	2.26	0.44
1:A:27:ARG:HG2	1:A:140:ARG:HH22	1.82	0.44
1:A:170:ARG:HB2	1:A:185:ILE:HG13	2.00	0.44
1:A:323:THR:HA	1:A:356:ASN:ND2	2.33	0.44
1:A:265:ASN:HD21	1:A:287:GLU:N	2.01	0.43
1:A:61:GLN:HE22	1:A:73:ILE:H	1.67	0.42
1:A:427:ILE:HG23	1:A:443:LEU:HD21	2.00	0.42
1:A:384:ILE:HD13	1:A:384:ILE:H	1.84	0.42
1:A:388:ASP:O	1:A:392:ILE:HG13	2.20	0.42
1:A:94:TRP:CZ3	1:A:242:ILE:HD11	2.52	0.42
1:A:79:GLU:H	1:A:79:GLU:CD	2.28	0.42
1:A:20:VAL:HG23	1:A:260:THR:HG22	2.02	0.41
1:A:164:ASN:HB3	1:A:191:THR:HG23	2.01	0.41
1:A:174:LEU:HD13	1:A:176:GLN:CG	2.51	0.41
1:A:132:SER:C	1:A:134:ASN:H	2.29	0.41
1:A:144:THR:HG23	1:A:281:LEU:HD11	2.02	0.41
1:A:122:ALA:HB2	1:A:185:ILE:HG22	2.02	0.41
1:A:231:GLN:HB2	1:A:234:THR:CG2	2.51	0.41
1:A:331:SER:OG	1:A:473:ILE:HG21	2.20	0.41
1:A:72:ILE:HG22	1:A:86:TRP:NE1	2.37	0.40
1:A:473:ILE:HD11	2:A:1772:HOH:O	2.21	0.40
1:A:129:GLU:OE1	1:A:248:ILE:HD11	2.22	0.40
1:A:79:GLU:HG2	1:A:80:GLU:OE1	2.22	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	486/511 (95%)	435 (90%)	36 (7%)	15 (3%)	3 5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	45	MET
1	A	219	SER
1	A	239	ASN
1	A	253	ASN
1	A	274	GLU
1	A	415	PHE
1	A	416	LYS
1	A	408	PHE
1	A	417	ALA
1	A	30	GLY
1	A	338	GLU
1	A	386	ALA
1	A	242	ILE
1	A	189	PRO

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	406/422 (96%)	362 (89%)	44 (11%)	6 13

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	18	THR
1	A	20	VAL
1	A	28	ILE
1	A	64	LEU
1	A	86	TRP
1	A	92	SER
1	A	93	PRO
1	A	97	GLU
1	A	106	LEU
1	A	140	ARG
1	A	143	VAL
1	A	144	THR
1	A	153	ILE
1	A	174	LEU
1	A	179	THR
1	A	182	MET
1	A	189	PRO
1	A	191	THR
1	A	196	ASP
1	A	205	ARG
1	A	208	THR
1	A	242	ILE
1	A	249	SER
1	A	266	HIS
1	A	288	ILE
1	A	291	SER
1	A	312	LYS
1	A	331	SER
1	A	343	LYS
1	A	349	ARG
1	A	366	TYR
1	A	373	ILE
1	A	377	MET
1	A	382	LEU
1	A	384	ILE
1	A	385	ASN
1	A	408	PHE
1	A	411	LEU
1	A	413	LYS
1	A	443	LEU
1	A	461	LEU

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Mol	Chain	Res	Type
1	A	504	GLU
1	A	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	134	ASN
1	A	145	GLN
1	A	164	ASN
1	A	180	GLN
1	A	231	GLN
1	A	239	ASN
1	A	264	ASN
1	A	265	ASN
1	A	292	ASN
1	A	302	ASN
1	A	314	GLN
1	A	356	ASN
1	A	385	ASN
1	A	394	ASN
1	A	400	ASN
1	A	406	ASN
1	A	425	ASN
1	A	426	ASN
1	A	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 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.