



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RH1  
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](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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

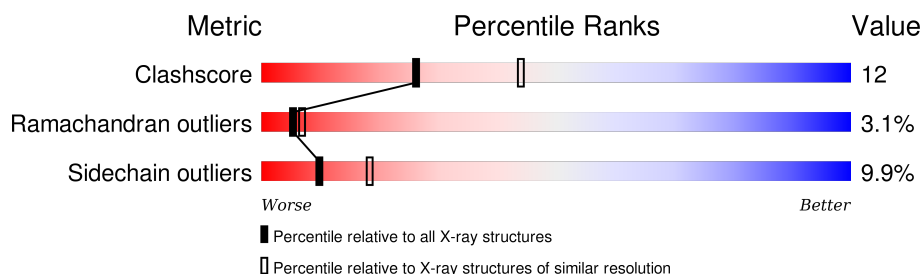
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	

## 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.

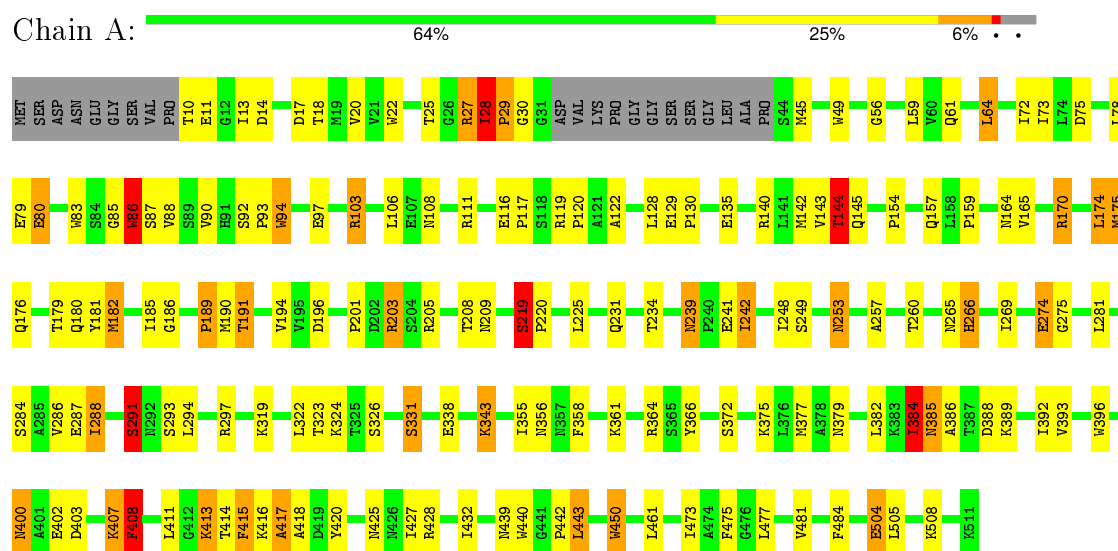
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total	O	0	0
			184	184		

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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: Colicin B



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.16Å 138.17Å 106.16Å 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 <sup>2</sup> )	12.0	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	0.79	2/3789 (0.1%)	1.51	49/5149 (1.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	GLU	CB-CG	5.70	1.62	1.52
1	A	49	TRP	CG-CD2	-5.04	1.35	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MET	CG-SD-CE	-9.85	84.44	100.20
1	A	119	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	86	TRP	CD1-CG-CD2	9.12	113.59	106.30
1	A	396	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	83	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	80	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	A	450	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	A	170	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	A	83	TRP	CE2-CD2-CG	-8.13	100.79	107.30
1	A	22	TRP	CD1-CG-CD2	8.09	112.78	106.30
1	A	396	TRP	CE2-CD2-CG	-8.06	100.86	107.30
1	A	94	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	440	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	86	TRP	CE2-CD2-CG	-7.87	101.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	22	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	49	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	94	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	A	450	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	A	85	GLY	CA-C-N	-7.05	101.68	117.20
1	A	49	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	364	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	103	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	119	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	418	ALA	CA-C-N	-6.36	103.22	117.20
1	A	407	LYS	CA-C-N	-6.19	103.58	117.20
1	A	407	LYS	C-N-CA	6.13	137.04	121.70
1	A	29	PRO	N-CA-C	5.95	127.57	112.10
1	A	103	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	90	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	A	415	PHE	C-N-CA	5.73	136.03	121.70
1	A	144	THR	CA-CB-CG2	5.66	120.32	112.40
1	A	219	SER	N-CA-CB	-5.58	102.12	110.50
1	A	440	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	A	253	ASN	N-CA-C	5.48	125.81	111.00
1	A	384	ILE	CB-CA-C	-5.46	100.69	111.60
1	A	111	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	80	GLU	CB-CG-CD	5.42	128.84	114.20
1	A	396	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A	83	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	A	291	SER	N-CA-C	5.30	125.32	111.00
1	A	17	ASP	CA-C-N	-5.23	105.70	117.20
1	A	86	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	407	LYS	O-C-N	5.13	130.90	122.70
1	A	440	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	A	181	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	A	364	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	396	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	80	GLU	CB-CA-C	5.06	120.52	110.40

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	91	0
2	A	184	0	0	3	0
All	All	3902	0	3701	91	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 12.

All (91) 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:HD22	1:A:385:ASN:H	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:10:THR:HG22	1:A:11:GLU:H	1.63	0.62
1:A:407:LYS:HB3	1:A:411:LEU:HD22	1.82	0.61
1:A:103:ARG:HH12	1:A:145:GLN:HE22	1.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:408:PHE:HA	1:A:414:THR:N	2.25	0.51
1:A:393:VAL:HG13	1:A:432:ILE:HG23	1.91	0.51
1:A:291:SER:HA	1:A:294:LEU:HD12	1.93	0.51
1:A:28:ILE:HD13	1:A:28:ILE:H	1.75	0.51
1:A:186:GLY:HA2	1:A:190:MET:HE1	1.91	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:288:ILE:H	1:A:288:ILE:HD12	1.79	0.48
1:A:25:THR:HB	1:A:293:SER:OG	2.13	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:408:PHE:O	1:A:413:LYS:HA	2.13	0.47
1:A:358:PHE:HA	1:A:361:LYS:HD2	1.95	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:322:LEU:HD22	1:A:355:ILE:O	2.16	0.46
1:A:116:GLU:HA	1:A:117:PRO:HD2	1.78	0.46
1:A:174:LEU:HD22	2:A:1367:HOH:O	2.15	0.45
1:A:182:MET:HE1	1:A:286:VAL:HG21	1.98	0.45
1:A:154:PRO:HD2	1:A:157:GLN:HB2	1.97	0.45
1:A:274:GLU:HG3	1:A:275:GLY:N	2.28	0.45
1:A:75:ASP:HB3	1:A:78:LEU:HB2	1.99	0.45
1:A:323:THR:HA	1:A:356:ASN:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:ND2	1:A:385:ASN:H	2.10	0.44
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: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: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:427:ILE:HG23	1:A:443:LEU:HD21	2.00	0.42
1:A:61:GLN:HE22	1:A:73:ILE:H	1.67	0.42
1:A:384:ILE:H	1:A:384:ILE:HD13	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: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:144:THR:HG23	1:A:281:LEU:HD11	2.02	0.41
1:A:231:GLN:HB2	1:A:234:THR:CG2	2.51	0.41
1:A:122:ALA:HB2	1:A:185:ILE:HG22	2.02	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%)	5 7

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%)	366 (90%)	40 (10%)	10	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	18	THR
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	108	ASN

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Mol	Chain	Res	Type
1	A	143	VAL
1	A	144	THR
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	203	ARG
1	A	205	ARG
1	A	208	THR
1	A	249	SER
1	A	266	HIS
1	A	288	ILE
1	A	291	SER
1	A	331	SER
1	A	343	LYS
1	A	366	TYR
1	A	377	MET
1	A	379	ASN
1	A	382	LEU
1	A	384	ILE
1	A	385	ASN
1	A	400	ASN
1	A	408	PHE
1	A	413	LYS
1	A	443	LEU
1	A	461	LEU
1	A	504	GLU
1	A	505	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	61	GLN
1	A	145	GLN
1	A	164	ASN
1	A	180	GLN
1	A	239	ASN
1	A	265	ASN
1	A	292	ASN

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Mol	Chain	Res	Type
1	A	356	ASN
1	A	379	ASN
1	A	385	ASN
1	A	394	ASN
1	A	400	ASN
1	A	425	ASN
1	A	426	ASN
1	A	507	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 carbohydrates 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 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.