



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FEW  
Title : Structure and Function of Colicin S4, a colicin with a duplicated receptor binding domain  
Authors : Arnold, T.; Linke, D.; Zeth, K.  
Deposited on : 2008-12-01  
Resolution : 2.45 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

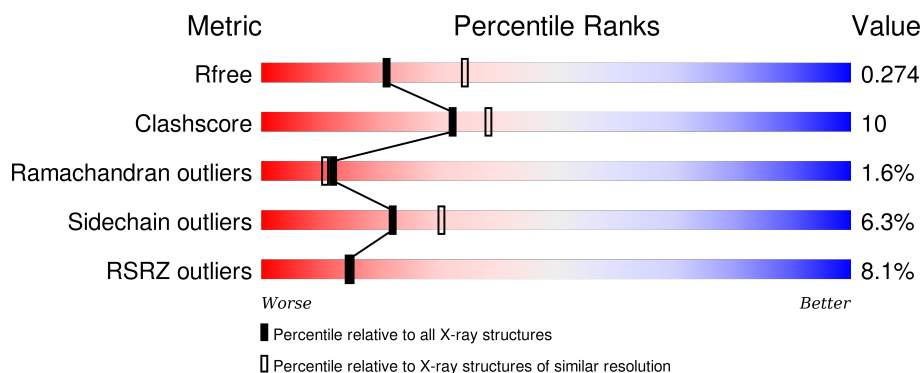
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

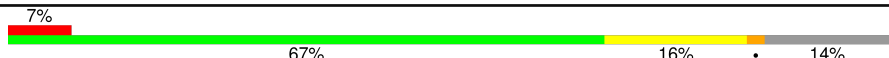
The reported resolution of this entry is 2.45 Å.

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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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.

Mol	Chain	Length	Quality of chain
1	X	505	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3587 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 S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	433	Total	C	N	O	S	0	6	0
			3386	2142	588	649	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	500	HIS	-	EXPRESSION TAG	UNP Q9XB47
X	501	HIS	-	EXPRESSION TAG	UNP Q9XB47
X	502	HIS	-	EXPRESSION TAG	UNP Q9XB47
X	503	HIS	-	EXPRESSION TAG	UNP Q9XB47
X	504	HIS	-	EXPRESSION TAG	UNP Q9XB47
X	505	HIS	-	EXPRESSION TAG	UNP Q9XB47

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Na	0	0
			1	1		

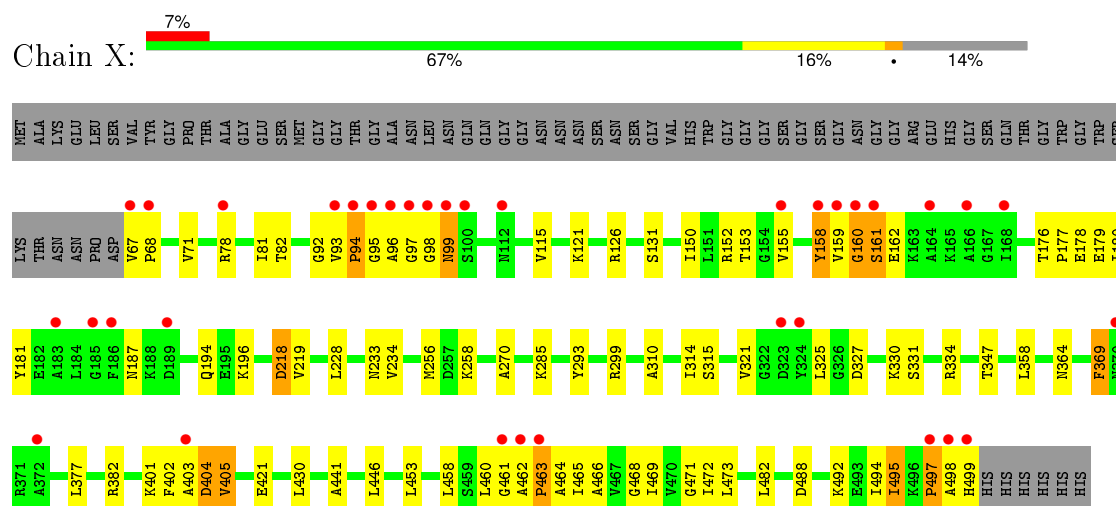
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	200	Total	O	0	0
			200	200		

### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: Colicin S4



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	240.34Å 240.34Å 80.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.45 36.93 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.45) 99.6 (36.93-2.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.218 , 0.258 0.250 , 0.274	Depositor DCC
$R_{free}$ test set	1614 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32297 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	X	0.54	0/3466	0.64	2/4687 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	405	VAL	N-CA-C	-5.48	96.21	111.00
1	X	218	ASP	CB-CG-OD1	5.36	123.12	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	X	3386	0	3374	71	0
2	X	1	0	0	0	0
3	X	200	0	0	2	1
All	All	3587	0	3374	71	1

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 10.

All (71) 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:X:92:GLY:CA	1:X:93:VAL:HG22	1.89	1.02
1:X:92:GLY:HA2	1:X:93:VAL:CG2	1.89	1.02
1:X:92:GLY:HA2	1:X:93:VAL:HG22	0.97	0.96
1:X:160:GLY:HA3	1:X:162:GLU:N	1.84	0.92
1:X:463:PRO:HB2	1:X:464:ALA:HA	1.52	0.89
1:X:402:PHE:HB2	1:X:404:ASP:H	1.38	0.88
1:X:96:ALA:N	1:X:97:GLY:HA2	1.92	0.84
1:X:258:LYS:HE3	3:X:671:HOH:O	1.79	0.82
1:X:99:ASN:HD22	1:X:99:ASN:H	1.32	0.78
1:X:402:PHE:HB2	1:X:404:ASP:N	1.97	0.78
1:X:152:ARG:HH22	1:X:187:ASN:HD21	1.33	0.75
1:X:402:PHE:N	1:X:403:ALA:HA	2.01	0.74
1:X:160:GLY:HA3	1:X:161:SER:C	2.07	0.74
1:X:472:ILE:HD12	1:X:494:ILE:HD13	1.69	0.73
1:X:96:ALA:H	1:X:97:GLY:HA2	1.52	0.73
1:X:95:GLY:H	1:X:96:ALA:HA	1.54	0.72
1:X:121:LYS:O	1:X:126:ARG:NH2	2.23	0.72
1:X:81:ILE:HD12	1:X:219:VAL:HG22	1.71	0.71
1:X:233:ASN:HD22	1:X:441:ALA:H	1.37	0.71
1:X:463:PRO:HB3	1:X:466:ALA:HB3	1.72	0.69
1:X:472:ILE:HD12	1:X:494:ILE:CD1	2.21	0.68
1:X:404:ASP:HB2	1:X:405:VAL:HA	1.78	0.65
1:X:96:ALA:H	1:X:97:GLY:CA	2.09	0.65
1:X:96:ALA:N	1:X:97:GLY:CA	2.60	0.64
1:X:462:ALA:N	1:X:463:PRO:HD3	2.14	0.63
1:X:404:ASP:CB	1:X:405:VAL:HA	2.29	0.63
1:X:99:ASN:ND2	1:X:99:ASN:H	1.96	0.62
1:X:95:GLY:N	1:X:96:ALA:HA	2.13	0.59
1:X:463:PRO:CB	1:X:464:ALA:HA	2.25	0.59
1:X:472:ILE:CD1	1:X:494:ILE:HD13	2.33	0.58
1:X:99:ASN:HD22	1:X:99:ASN:N	1.97	0.58
1:X:233:ASN:ND2	1:X:441:ALA:H	2.02	0.57
1:X:176:THR:HG22	1:X:179:GLU:OE2	2.04	0.57
1:X:176:THR:OG1	1:X:177:PRO:HD2	2.04	0.57
1:X:234:VAL:HG21	1:X:285:LYS:HG2	1.86	0.57
1:X:446:LEU:HD11	1:X:482:LEU:HD11	1.88	0.56
1:X:463:PRO:CB	1:X:466:ALA:HB3	2.36	0.54
1:X:325:LEU:HD21	1:X:472:ILE:HD11	1.91	0.53
1:X:178:GLU:HA	1:X:181:TYR:CD2	2.44	0.52
1:X:402:PHE:HE2	1:X:405:VAL:HG23	1.76	0.51
1:X:463:PRO:HB2	1:X:464:ALA:CA	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:293:TYR:CE1	1:X:299:ARG:HG2	2.47	0.50
1:X:93:VAL:N	1:X:94:PRO:HD3	2.27	0.50
1:X:334:ARG:HG3	1:X:334:ARG:HH11	1.77	0.49
1:X:347:THR:HG23	3:X:577:HOH:O	2.11	0.49
1:X:310:ALA:O	1:X:314:ILE:HG12	2.13	0.49
1:X:93:VAL:C	1:X:95:GLY:HA3	2.34	0.48
1:X:152:ARG:HH12	1:X:187:ASN:ND2	2.12	0.47
1:X:150:ILE:HD13	1:X:194:GLN:HG2	1.96	0.47
1:X:67:VAL:N	1:X:68:PRO:HA	2.30	0.47
1:X:468:GLY:O	1:X:472:ILE:HG12	2.15	0.46
1:X:466:ALA:HA	1:X:469:ILE:HD12	1.96	0.46
1:X:369:PHE:CD2	1:X:369:PHE:N	2.84	0.46
1:X:461:GLY:HA2	1:X:462:ALA:HB2	1.96	0.46
1:X:256:MET:HE1	1:X:270:ALA:HB3	1.98	0.46
1:X:401:LYS:C	1:X:403:ALA:HA	2.36	0.46
1:X:177:PRO:HA	1:X:180:ILE:HD12	1.98	0.45
1:X:498:ALA:HA	1:X:499:HIS:HA	1.66	0.45
1:X:382:ARG:NH2	1:X:421:GLU:OE2	2.50	0.45
1:X:404:ASP:CB	1:X:405:VAL:CA	2.97	0.43
1:X:327:ASP:HA	1:X:330:LYS:HB2	2.01	0.42
1:X:97:GLY:CA	1:X:99:ASN:HA	2.49	0.42
1:X:402:PHE:HD2	1:X:405:VAL:HB	1.85	0.42
1:X:78[B]:ARG:HH22	1:X:218:ASP:CB	2.33	0.41
1:X:93:VAL:O	1:X:95:GLY:HA3	2.20	0.41
1:X:97:GLY:HA2	1:X:98:GLY:HA3	1.75	0.41
1:X:364:ASN:ND2	1:X:495:ILE:HG21	2.36	0.41
1:X:497:PRO:HB2	1:X:498:ALA:H	1.71	0.41
1:X:488:ASP:O	1:X:492:LYS:HB2	2.20	0.41
1:X:321:VAL:HG11	1:X:471:GLY:HA3	2.02	0.40

All (1) 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)
3:X:566:HOH:O	3:X:662:HOH:O[2_655]	2.19	0.01



## 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	X	437/505 (86%)	406 (93%)	23 (5%)	8 (2%)	11 9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	158[A]	TYR
1	X	158[B]	TYR
1	X	159	VAL
1	X	161	SER
1	X	160	GLY
1	X	497	PRO
1	X	94	PRO
1	X	463	PRO

### 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	X	357/404 (88%)	335 (94%)	22 (6%)	23 31

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	71	VAL
1	X	82	THR
1	X	99	ASN

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Mol	Chain	Res	Type
1	X	115	VAL
1	X	131	SER
1	X	153	THR
1	X	155	VAL
1	X	196	LYS
1	X	228	LEU
1	X	315	SER
1	X	331	SER
1	X	358	LEU
1	X	369	PHE
1	X	377	LEU
1	X	404	ASP
1	X	430	LEU
1	X	453	LEU
1	X	458	LEU
1	X	460	LEU
1	X	465	ILE
1	X	473	LEU
1	X	495	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	99	ASN
1	X	103	GLN
1	X	187	ASN
1	X	233	ASN
1	X	303	GLN
1	X	342	ASN
1	X	370	ASN
1	X	387	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	433/505 (85%)	0.58	35 (8%) 15 15	19, 51, 72, 86	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	67	VAL	8.2
1	X	96	ALA	8.1
1	X	499	HIS	7.6
1	X	498	ALA	6.9
1	X	463	PRO	6.3
1	X	98	GLY	6.0
1	X	497	PRO	5.8
1	X	403	ALA	5.7
1	X	164	ALA	5.1
1	X	462	ALA	5.0
1	X	161	SER	4.5
1	X	158[A]	TYR	4.4
1	X	97	GLY	4.3
1	X	160	GLY	3.9
1	X	324	TYR	3.8
1	X	159	VAL	3.5
1	X	99	ASN	3.5
1	X	168	ILE	3.5
1	X	155	VAL	3.3
1	X	95	GLY	3.2
1	X	94	PRO	2.9
1	X	370	ASN	2.9
1	X	100	SER	2.8
1	X	323	ASP	2.8
1	X	372	ALA	2.7
1	X	189	ASP	2.7
1	X	166	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	112	ASN	2.5
1	X	185	GLY	2.4
1	X	461	GLY	2.4
1	X	183	ALA	2.3
1	X	78[A]	ARG	2.2
1	X	68	PRO	2.2
1	X	93	VAL	2.1
1	X	186	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	X	506	1/1	0.67	0.34	-	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.