



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:28 am GMT

PDB ID : 4RMO  
Title : Crystal Structure of the CptIN Type III Toxin-Antitoxin System from *Eubacterium rectale*  
Authors : Rao, F.; Voss, J.E.; Short, F.L.; Luisi, B.F.  
Deposited on : 2014-10-21  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

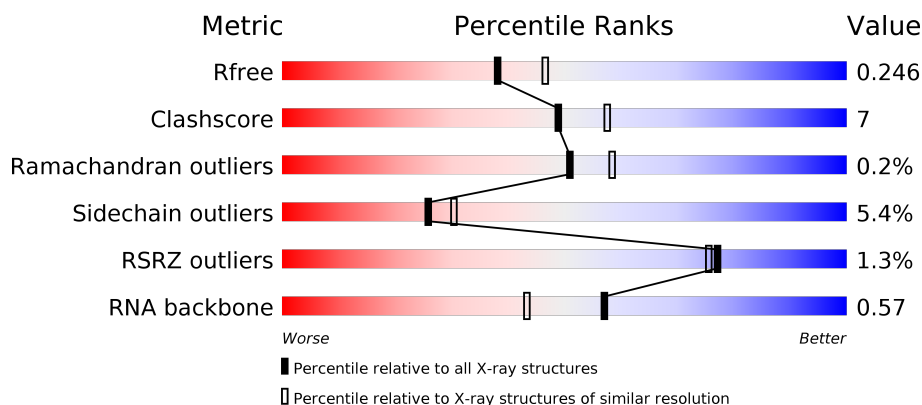
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)
RNA backbone	2435	1007 (2.74-1.66)

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	A	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 10%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 80%; margin: 0 auto;"> <span>85%</span> <span>12%</span> </div> </div>
1	C	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 84%, yellow 15%, orange 1%, red 1%);"></div> <div style="display: flex; justify-content: space-between; width: 80%; margin: 0 auto;"> <span>84%</span> <span>15%</span> </div> </div>
1	E	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 10%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 80%; margin: 0 auto;"> <span>81%</span> <span>15%</span> </div> </div>
1	G	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 83%, yellow 15%, orange 2%, red 2%);"></div> <div style="display: flex; justify-content: space-between; width: 80%; margin: 0 auto;"> <span>83%</span> <span>15%</span> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	155	
1	K	155	
1	M	155	
1	O	155	
2	B	45	
2	D	45	
2	F	45	
2	H	45	
2	J	45	
2	L	45	
2	N	45	
2	P	45	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	G	201	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19477 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 CptN Toxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			
1	C	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			
1	E	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			
1	G	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			
1	I	155	Total	C	N	O	S	Se	0	1	0
			1293	827	226	233	2	5			
1	K	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			
1	M	155	Total	C	N	O	S	Se	0	1	0
			1300	830	229	234	2	5			
1	O	155	Total	C	N	O	S	Se	0	1	0
			1303	832	230	234	2	5			

- Molecule 2 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			
2	D	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			
2	F	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			
2	H	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			
2	J	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			
2	L	45	Total	C	N	O	P	0	0	0
			962	430	171	316	45			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	45	Total 962	C 430	N 171	O 316	P 45	0	0	0
2	P	45	Total 962	C 430	N 171	O 316	P 45	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	3	Total 3	Ca 3	0	0
3	G	1	Total 1	Ca 1	0	0
3	J	6	Total 6	Ca 6	0	0
3	D	6	Total 6	Ca 6	0	0
3	K	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	H	6	Total 6	Ca 6	0	0
3	B	5	Total 5	Ca 5	0	0
3	I	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	N	5	Total 5	Ca 5	0	0
3	O	1	Total 1	Ca 1	0	0
3	L	5	Total 5	Ca 5	0	0
3	F	4	Total 4	Ca 4	0	0
3	M	1	Total 1	Ca 1	0	0

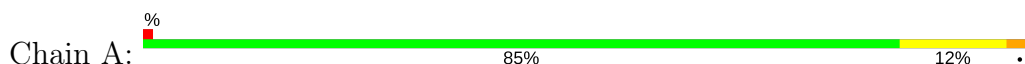
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total 82	O 82	0	0
4	B	99	Total 99	O 99	0	0
4	C	88	Total 88	O 88	0	0
4	D	98	Total 98	O 98	0	0
4	E	53	Total 53	O 53	0	0
4	F	67	Total 67	O 67	0	0
4	G	112	Total 112	O 112	0	0
4	H	100	Total 100	O 100	0	0
4	I	81	Total 81	O 81	0	0
4	J	100	Total 100	O 100	0	0
4	K	89	Total 89	O 89	0	0
4	L	85	Total 85	O 85	0	0
4	M	54	Total 54	O 54	0	0
4	N	83	Total 83	O 83	0	0
4	O	67	Total 67	O 67	0	0
4	P	64	Total 64	O 64	0	0

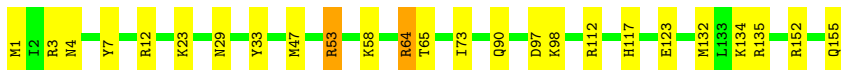
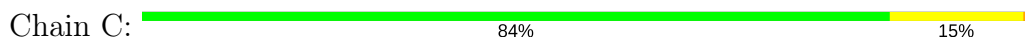
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

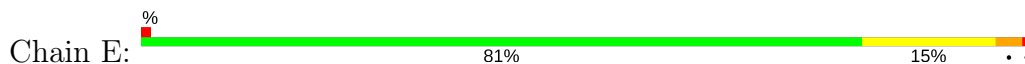
- Molecule 1: CptN Toxin



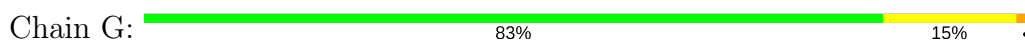
- Molecule 1: CptN Toxin



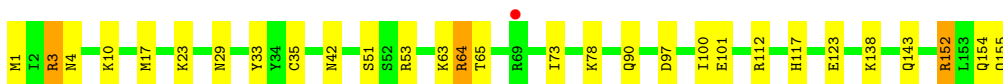
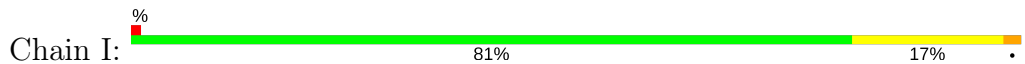
- Molecule 1: CptN Toxin



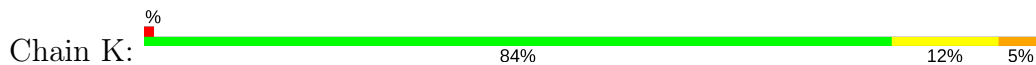
- Molecule 1: CptN Toxin



- Molecule 1: CptN Toxin

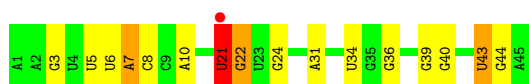


- Molecule 1: CptN Toxin









- Molecule 2: RNA (45-MER)



- Molecule 2: RNA (45-MER)



- Molecule 2: RNA (45-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.11Å 185.89Å 138.78Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	63.12 – 2.20 63.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (63.12-2.20) 97.8 (63.04-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.199 , 0.234 0.212 , 0.246	Depositor DCC
$R_{free}$ test set	7919 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A23

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	0.84	4/1331 (0.3%)	0.92	4/1776 (0.2%)
1	C	0.86	0/1331	1.01	12/1776 (0.7%)
1	E	0.81	2/1331 (0.2%)	0.94	7/1776 (0.4%)
1	G	0.90	5/1331 (0.4%)	0.95	5/1776 (0.3%)
1	I	0.85	0/1321	0.91	3/1764 (0.2%)
1	K	0.90	5/1331 (0.4%)	1.03	8/1776 (0.5%)
1	M	0.87	6/1328 (0.5%)	0.94	7/1773 (0.4%)
1	O	0.80	2/1331 (0.2%)	0.90	7/1776 (0.4%)
2	B	0.67	1/1048 (0.1%)	0.98	3/1632 (0.2%)
2	D	0.60	0/1048	0.92	4/1632 (0.2%)
2	F	0.54	0/1048	0.91	4/1632 (0.2%)
2	H	0.51	0/1048	0.90	3/1632 (0.2%)
2	J	0.72	1/1048 (0.1%)	0.98	6/1632 (0.4%)
2	L	0.58	0/1048	0.92	5/1632 (0.3%)
2	N	0.64	0/1048	0.98	6/1632 (0.4%)
2	P	0.76	3/1048 (0.3%)	1.33	18/1632 (1.1%)
All	All	0.76	29/19019 (0.2%)	0.97	102/27249 (0.4%)

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	0	1
1	K	0	1
1	O	0	1
2	B	0	1
2	D	0	1
2	H	0	1
2	P	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	42	U	O3'-P	-10.66	1.48	1.61
2	P	19	U	O3'-P	8.94	1.71	1.61
2	P	44	G	O5'-C5'	-7.43	1.30	1.42
2	J	40	G	O5'-C5'	-6.01	1.33	1.42
1	M	123[A]	GLU	CD-OE1	5.83	1.32	1.25

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	44	G	O5'-P-OP1	-16.77	90.58	110.70
2	B	42	U	C2'-C3'-O3'	14.73	141.91	109.50
2	P	44	G	O5'-P-OP2	11.68	124.71	110.70
2	P	44	G	C5'-C4'-O4'	-11.51	95.29	109.10
2	P	38	C	C2'-C3'-O3'	11.06	133.83	109.50

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	GLN	Peptide
2	B	44	G	Sidechain
2	D	44	G	Sidechain
2	H	44	G	Sidechain
1	K	154	GLN	Peptide

## 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	A	1303	0	1315	23	0
1	C	1303	0	1315	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1303	0	1315	22	0
1	G	1303	0	1315	17	0
1	I	1293	0	1289	22	0
1	K	1303	0	1315	19	0
1	M	1300	0	1306	28	0
1	O	1303	0	1315	12	0
2	B	962	0	481	11	0
2	D	962	0	481	13	0
2	F	962	0	481	13	0
2	H	962	0	481	12	0
2	J	962	0	481	12	0
2	L	962	0	481	16	0
2	N	962	0	481	14	0
2	P	962	0	481	20	0
3	A	1	0	0	0	0
3	B	5	0	0	0	0
3	C	1	0	0	0	0
3	D	6	0	0	0	0
3	E	1	0	0	0	0
3	F	4	0	0	0	0
3	G	1	0	0	0	0
3	H	6	0	0	0	0
3	I	1	0	0	0	0
3	J	6	0	0	0	0
3	K	1	0	0	0	0
3	L	5	0	0	0	0
3	M	1	0	0	0	0
3	N	5	0	0	1	0
3	O	1	0	0	0	0
3	P	3	0	0	0	0
4	A	82	0	0	3	1
4	B	99	0	0	2	0
4	C	88	0	0	2	1
4	D	98	0	0	1	0
4	E	53	0	0	1	0
4	F	67	0	0	4	0
4	G	112	0	0	8	0
4	H	100	0	0	4	0
4	I	81	0	0	4	0
4	J	100	0	0	5	0
4	K	89	0	0	4	0
4	L	85	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	54	0	0	12	0
4	N	83	0	0	9	0
4	O	67	0	0	1	0
4	P	64	0	0	4	0
All	All	19477	0	14333	221	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 7.

The worst 5 of 221 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)
2:L:18:A:N7	4:L:212:HOH:O	1.58	1.32
1:M:53:ARG:CD	4:M:349:HOH:O	1.77	1.28
1:M:53:ARG:NE	4:M:349:HOH:O	1.67	1.21
2:N:10:A:OP2	4:N:261:HOH:O	1.66	1.13
1:A:1:MSE:HE3	1:A:7:TYR:CD2	1.93	1.04

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)
4:A:326:HOH:O	4:C:377:HOH:O[1_455]	2.13	0.07

## 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	154/155 (99%)	148 (96%)	5 (3%)	1 (1%)	28 29
1	C	154/155 (99%)	150 (97%)	4 (3%)	0	100 100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
1	G	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
1	I	154/155 (99%)	151 (98%)	3 (2%)	0	100	100
1	K	154/155 (99%)	149 (97%)	4 (3%)	1 (1%)	28	29
1	M	154/155 (99%)	150 (97%)	4 (3%)	0	100	100
1	O	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
All	All	1232/1240 (99%)	1195 (97%)	35 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	K	154	GLN

### 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	143/137 (104%)	135 (94%)	8 (6%)	25	29
1	C	143/137 (104%)	137 (96%)	6 (4%)	34	43
1	E	143/137 (104%)	132 (92%)	11 (8%)	15	15
1	G	143/137 (104%)	137 (96%)	6 (4%)	34	43
1	I	139/137 (102%)	131 (94%)	8 (6%)	23	27
1	K	143/137 (104%)	132 (92%)	11 (8%)	15	15
1	M	142/137 (104%)	134 (94%)	8 (6%)	25	29
1	O	143/137 (104%)	132 (92%)	11 (8%)	15	15
All	All	1139/1096 (104%)	1070 (94%)	69 (6%)	26	25

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	3	ARG
1	I	152	ARG
1	O	101	GLU
1	I	65	THR
1	I	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	117	HIS
1	I	25	ASN
1	K	155	GLN
1	G	25	ASN
1	G	29	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	44/45 (97%)	6 (13%)	0
2	D	44/45 (97%)	5 (11%)	0
2	F	44/45 (97%)	4 (9%)	0
2	H	44/45 (97%)	4 (9%)	0
2	J	44/45 (97%)	6 (13%)	0
2	L	44/45 (97%)	5 (11%)	0
2	N	44/45 (97%)	5 (11%)	0
2	P	44/45 (97%)	10 (22%)	0
All	All	352/360 (97%)	45 (12%)	0

5 of 45 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	U
2	B	10	A
2	B	21	U
2	B	22	G
2	B	31	A

There are no RNA pucker outliers to report.



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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	A23	B	45	2	19,28,29	1.58	4 (21%)	20,43,46	2.04	5 (25%)
2	A23	D	45	2	19,28,29	1.42	4 (21%)	20,43,46	1.56	4 (20%)
2	A23	F	45	2	19,28,29	1.16	1 (5%)	20,43,46	1.63	4 (20%)
2	A23	H	45	2	19,28,29	1.01	2 (10%)	20,43,46	1.68	3 (15%)
2	A23	J	45	2	19,28,29	0.98	1 (5%)	20,43,46	1.74	4 (20%)
2	A23	L	45	2	19,28,29	1.76	4 (21%)	20,43,46	2.82	10 (50%)
2	A23	N	45	2	19,28,29	1.22	2 (10%)	20,43,46	2.25	5 (25%)
2	A23	P	45	2	19,28,29	1.13	2 (10%)	20,43,46	2.00	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A23	B	45	2	-	0/3/35/36	0/4/4/4
2	A23	D	45	2	-	0/3/35/36	0/4/4/4
2	A23	F	45	2	-	0/3/35/36	0/4/4/4
2	A23	H	45	2	-	0/3/35/36	0/4/4/4
2	A23	J	45	2	-	0/3/35/36	0/4/4/4
2	A23	L	45	2	-	0/3/35/36	0/4/4/4
2	A23	N	45	2	-	0/3/35/36	0/4/4/4
2	A23	P	45	2	-	0/3/35/36	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	45	A23	C4-N3	-3.44	1.30	1.35
2	L	45	A23	C2-N3	-3.31	1.26	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	45	A23	O5'-C5'	-2.77	1.40	1.44
2	F	45	A23	O5'-C5'	-2.74	1.40	1.44
2	B	45	A23	O2'-C2'	-2.65	1.39	1.45

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	45	A23	N3-C2-N1	-7.15	122.63	128.86
2	B	45	A23	N3-C2-N1	-5.70	123.89	128.86
2	P	45	A23	N3-C2-N1	-5.54	124.03	128.86
2	J	45	A23	N3-C2-N1	-4.53	124.91	128.86
2	F	45	A23	N3-C2-N1	-4.43	125.00	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	45	A23	1	0
2	L	45	A23	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are 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 [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 ⓘ

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	A	150/155 (96%)	-0.21	1 (0%) 87 86	21, 33, 62, 74	0
1	C	150/155 (96%)	-0.11	0 100 100	21, 34, 66, 89	0
1	E	150/155 (96%)	0.01	1 (0%) 87 86	27, 47, 77, 94	0
1	G	150/155 (96%)	-0.01	0 100 100	18, 30, 57, 76	0
1	I	150/155 (96%)	-0.02	1 (0%) 87 86	20, 35, 67, 104	0
1	K	150/155 (96%)	-0.06	1 (0%) 87 86	21, 32, 61, 67	0
1	M	150/155 (96%)	0.03	2 (1%) 77 75	24, 40, 70, 90	0
1	O	150/155 (96%)	0.36	10 (6%) 19 17	25, 48, 97, 134	0
2	B	44/45 (97%)	-0.50	0 100 100	26, 32, 46, 86	0
2	D	44/45 (97%)	-0.29	0 100 100	22, 34, 49, 89	0
2	F	44/45 (97%)	-0.37	0 100 100	26, 40, 63, 98	0
2	H	44/45 (97%)	-0.36	0 100 100	25, 41, 60, 93	0
2	J	44/45 (97%)	-0.31	1 (2%) 61 58	23, 34, 48, 97	0
2	L	44/45 (97%)	-0.21	0 100 100	28, 39, 75, 102	0
2	N	44/45 (97%)	-0.21	0 100 100	24, 39, 65, 96	0
2	P	44/45 (97%)	0.44	3 (6%) 18 17	27, 55, 88, 111	0
All	All	1552/1600 (97%)	-0.05	20 (1%) 77 75	18, 38, 73, 134	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	67	LYS	5.8
1	K	41	TYR	4.2
1	M	41	TYR	3.6
1	O	129	VAL	3.1
1	O	66	GLY	2.9

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	A23	J	45	25/26	0.98	0.15	-	20,23,26,28	0
2	A23	P	45	25/26	0.98	0.12	-	23,27,31,34	0
2	A23	D	45	25/26	0.99	0.15	-	18,21,24,28	0
2	A23	F	45	25/26	0.98	0.12	-	20,23,27,27	0
2	A23	L	45	25/26	0.96	0.15	-	24,29,39,50	0
2	A23	B	45	25/26	0.94	0.12	-	40,47,53,58	0
2	A23	H	45	25/26	0.99	0.11	-	24,25,28,29	0
2	A23	N	45	25/26	0.98	0.10	-	27,32,36,40	0

## 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
3	CA	G	201	1/1	0.80	0.30	13.28	44,44,44,44	0
3	CA	E	201	1/1	0.99	0.11	0.65	29,29,29,29	0
3	CA	O	201	1/1	0.98	0.11	-0.71	34,34,34,34	0
3	CA	K	201	1/1	0.99	0.10	-0.75	29,29,29,29	0
3	CA	A	201	1/1	0.98	0.09	-1.45	33,33,33,33	0
3	CA	F	104	1/1	0.96	0.09	-2.66	49,49,49,49	0
3	CA	M	201	1/1	0.97	0.08	-3.20	41,41,41,41	0
3	CA	C	201	1/1	0.98	0.07	-3.39	40,40,40,40	0
3	CA	I	201	1/1	0.96	0.09	-3.65	44,44,44,44	0
3	CA	L	103	1/1	0.99	0.06	-7.65	65,65,65,65	0
3	CA	P	103	1/1	0.53	0.11	-	87,87,87,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	H	106	1/1	0.96	0.07	-	55,55,55,55	0
3	CA	N	105	1/1	0.97	0.08	-	63,63,63,63	0
3	CA	N	102	1/1	0.94	0.06	-	45,45,45,45	0
3	CA	B	103	1/1	0.98	0.10	-	41,41,41,41	0
3	CA	H	102	1/1	0.93	0.06	-	61,61,61,61	0
3	CA	L	105	1/1	0.88	0.09	-	78,78,78,78	0
3	CA	J	101	1/1	0.96	0.10	-	52,52,52,52	0
3	CA	D	102	1/1	0.95	0.05	-	51,51,51,51	0
3	CA	H	101	1/1	0.96	0.05	-	61,61,61,61	0
3	CA	J	105	1/1	0.94	0.11	-	70,70,70,70	0
3	CA	N	104	1/1	0.94	0.05	-	51,51,51,51	0
3	CA	F	103	1/1	0.98	0.07	-	53,53,53,53	0
3	CA	P	102	1/1	0.92	0.08	-	65,65,65,65	0
3	CA	D	104	1/1	0.86	0.45	-	100,100,100,100	0
3	CA	J	104	1/1	0.84	0.39	-	110,110,110,110	0
3	CA	J	106	1/1	0.96	0.05	-	58,58,58,58	0
3	CA	P	101	1/1	0.93	0.06	-	62,62,62,62	0
3	CA	D	103	1/1	0.96	0.06	-	38,38,38,38	0
3	CA	L	101	1/1	0.93	0.06	-	66,66,66,66	0
3	CA	N	101	1/1	0.98	0.06	-	54,54,54,54	0
3	CA	D	106	1/1	0.96	0.06	-	64,64,64,64	0
3	CA	H	104	1/1	0.97	0.03	-	66,66,66,66	0
3	CA	B	102	1/1	0.96	0.06	-	55,55,55,55	0
3	CA	H	103	1/1	0.93	0.06	-	63,63,63,63	0
3	CA	D	105	1/1	0.98	0.06	-	47,47,47,47	0
3	CA	B	105	1/1	0.97	0.06	-	69,69,69,69	0
3	CA	J	102	1/1	0.92	0.08	-	58,58,58,58	0
3	CA	H	105	1/1	0.99	0.06	-	43,43,43,43	0
3	CA	B	101	1/1	0.98	0.06	-	50,50,50,50	0
3	CA	F	102	1/1	0.94	0.07	-	62,62,62,62	0
3	CA	D	101	1/1	0.96	0.05	-	63,63,63,63	0
3	CA	F	101	1/1	0.90	0.10	-	70,70,70,70	0
3	CA	N	103	1/1	0.94	0.39	-	72,72,72,72	0
3	CA	B	104	1/1	0.95	0.04	-	61,61,61,61	0
3	CA	L	104	1/1	0.90	0.06	-	68,68,68,68	0
3	CA	J	103	1/1	0.99	0.06	-	36,36,36,36	0
3	CA	L	102	1/1	0.95	0.11	-	64,64,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.