



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 01:41 PM BST

PDB ID : 6BBA  
Title : Crystal structure of human mitochondrial ClpP complex with acyldepsipeptide ADEP-28  
Authors : Mabanglo, M.F.; Houry, W.A.  
Deposited on : 2017-10-17  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

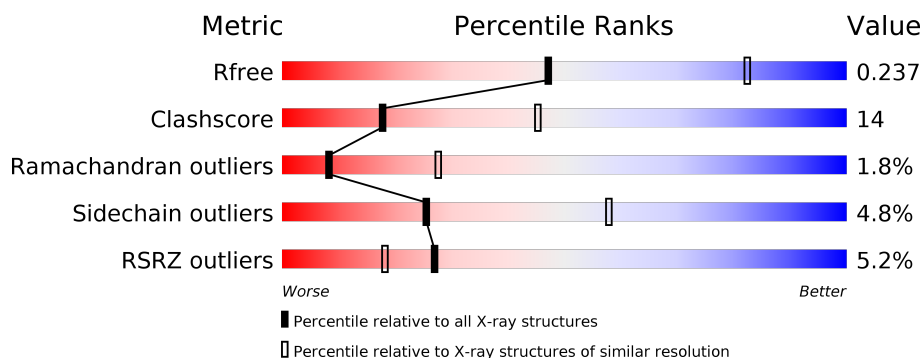
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	221	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	221	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	221	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>18%</div> <div>5%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	221	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	E	221	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>•</div> <div>15%</div> </div> </div>
1	F	221	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	221	
2	H	7	
2	I	7	
2	J	7	
2	K	7	
2	L	7	
2	M	7	
2	N	7	

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
2	ALO	I	3	-	-	X	-
2	ALO	K	3	-	-	X	-
2	ALO	N	3	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10836 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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1464	929	252	270	13			
1	B	185	Total	C	N	O	S	0	0	0
			1440	914	248	265	13			
1	C	189	Total	C	N	O	S	0	0	0
			1468	931	252	272	13			
1	D	189	Total	C	N	O	S	0	0	0
			1468	931	252	272	13			
1	E	188	Total	C	N	O	S	0	0	0
			1460	927	251	269	13			
1	F	190	Total	C	N	O	S	0	1	0
			1476	936	254	272	14			
1	G	188	Total	C	N	O	S	0	0	0
			1460	927	251	269	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q16740
B	57	SER	-	expression tag	UNP Q16740
C	57	SER	-	expression tag	UNP Q16740
D	57	SER	-	expression tag	UNP Q16740
E	57	SER	-	expression tag	UNP Q16740
F	57	SER	-	expression tag	UNP Q16740
G	57	SER	-	expression tag	UNP Q16740

- Molecule 2 is a protein called Acyldepsipeptide ADEP-28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	J	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	K	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	L	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	M	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	N	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	22	Total	O	0	0
			22	22		
3	C	22	Total	O	0	0
			22	22		
3	D	35	Total	O	0	0
			35	35		
3	E	38	Total	O	0	0
			38	38		
3	F	38	Total	O	0	0
			38	38		
3	G	30	Total	O	0	0
			30	30		
3	I	2	Total	O	0	0
			2	2		
3	M	1	Total	O	0	0
			1	1		
3	N	1	Total	O	0	0
			1	1		

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 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 ( $\text{RSRZ} > 2$ ). 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.

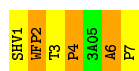
- Chain A:
- 
- 5% 63% 21% 14%
- Sequence logo for Chain A, showing conservation across 233 positions. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows amino acid positions. A bar chart at the top indicates the percentage of positions in each conservation bin: 5% (red), 63% (green), 21% (yellow), and 14% (grey). Red dots above the sequence indicate positions with high conservation (bits > 0.10).
- Key residues (positions and amino acids) shown in the sequence logo:
- 1236: I236
  - 1240: E240
  - 1243: K243
  - 1244: L244
  - 1245: K245
  - 1246: K246
  - 1247: Q247
  - 1248: L248
  - 1249: Y249
  - 1259: S259
  - 1262: V262
  - 1265: S265
  - 1266: A266
  - 1267: M267
  - 1271: R271
  - 1272: V272
  - 1273: K273
  - 1274: S274
  - 1275: P275
  - 1276: M276
  - 1277: E277
  - 1286: K286
  - 1287: V287
  - 1288: L288
  - 1289: V289
  - 1293: Q293
  - 1295: D295
  - 1296: GLY
  - 1297: GLU
  - 1298: ASP
  - 1299: GLU
  - 1300: GLU
  - 1301: PRO
  - 1302: THR
  - 1303: LEU
  - 1304: VAL
  - 1305: GLN
  - 1306: LYS
  - 1307: GLU
  - 1308: PRO
  - 1309: VAL
  - 1310: GLU
  - 1311: ALA
  - 1312: ALA
  - 1313: PRO
  - 1314: ALA
  - 1315: ALA
  - 1316: ALA
  - 1317: PRO
  - 1318: GLU
  - 1319: PRO
  - 1320: VAL
  - 1321: PRO
  - 1322: PRO
  - 1323: PRO
  - 1324: I234
  - 1325: C235

- Chain B:
- 
- | Residue Type | Count |
|--------------|-------|
| ASP          | 1     |
| ILE          | 1     |
| A235         | 1     |
| E240         | 1     |
| Q247         | 1     |
| I251         | 1     |
| S259         | 1     |
| L260         | 1     |
| G261         | 1     |
| V262         | 1     |
| I263         | 1     |
| E264         | 1     |
| E268         | 1     |
| R269         | 1     |
| D270         | 1     |
| R271         | 1     |
| Y272         | 1     |
| M276         | 1     |
| E277         | 1     |
| D285         | 1     |
| K286         | 1     |
| Y287         | 1     |
| L288         | 1     |
| P291         | 1     |
| P292         | 1     |
| Q293         | 1     |
| D294         | 1     |
| GLY          | 1     |
| GLU          | 1     |
| ASP          | 1     |
| GLU          | 1     |
| PRO          | 1     |
| THR          | 1     |
| LEU          | 1     |
| VAL          | 1     |
| GLN          | 1     |
| LYS          | 1     |
| GLU          | 1     |
| PRO          | 1     |
| VAL          | 1     |
| GLU          | 1     |
| ALA          | 1     |
| ALA          | 1     |
| PRO          | 1     |
| ALA          | 1     |
| ALA          | 1     |
| GLU          | 1     |
| ALA          | 1     |
| ARG          | 1     |
| GLY          | 1     |
| GLN          | 1     |
| ALA          | 1     |
| THR          | 1     |

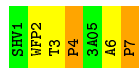
- Chain C:
- 
- 6% 62% 18% 5% 14%
- | Position   | 1   | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   | 11   | 12   | 13   | 14   | 15   | 16   | 17   | 18   | 19   | 20   |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |      |      |      |
|------------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|
| Amino Acid | S57 | V106 | E107 | Q108 | T109 | G110 | R111 | G112 | E113 | R114 | A115 | Y116 | L141 | Q150 | P157 | A174 | D177 | I182 | L183 | N184 | P186 | I186 | W189 | C190 | S196 | M197 | T206 | H211 | S212 | L213 | P214 | M219 | T220 | H221 | Q222 | P223 | S224 | GLY | GLY | ALA | ALA | ARG | GLY | ALA | G1N | A231 | T232 | P232 |

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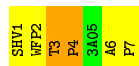
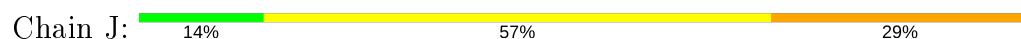




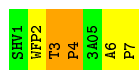
- Molecule 2: Acyldepsipeptide ADEP-28



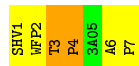
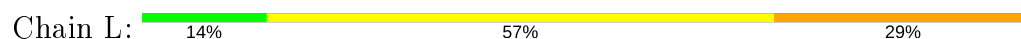
- Molecule 2: Acyldepsipeptide ADEP-28



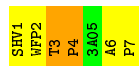
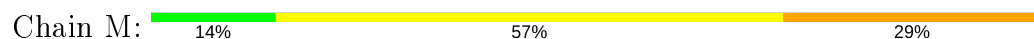
- Molecule 2: Acyldepsipeptide ADEP-28



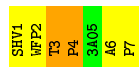
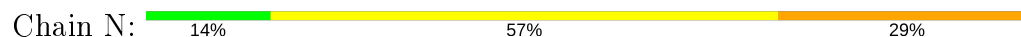
- Molecule 2: Acyldepsipeptide ADEP-28



- Molecule 2: Acyldepsipeptide ADEP-28



- Molecule 2: Acyldepsipeptide ADEP-28





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.40Å 172.40Å 135.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.73 – 2.80 46.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.73-2.80) 99.8 (46.73-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.187 , 0.235 0.190 , 0.237	Depositor DCC
$R_{free}$ test set	2017 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: ALO, WFP, 3A0, SHV

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	0.48	0/1490	0.63	0/2016
1	B	0.42	0/1466	0.58	0/1983
1	C	0.47	0/1494	0.61	0/2022
1	D	0.46	0/1494	0.67	0/2022
1	E	0.49	0/1486	0.61	0/2011
1	F	0.49	0/1505	0.64	0/2036
1	G	0.47	0/1486	0.62	0/2011
2	H	6.20	7/19 (36.8%)	1.23	0/24
2	I	6.16	7/19 (36.8%)	1.41	0/24
2	J	6.15	7/19 (36.8%)	1.24	0/24
2	K	6.13	7/19 (36.8%)	1.71	0/24
2	L	6.14	7/19 (36.8%)	1.26	0/24
2	M	6.00	7/19 (36.8%)	1.78	0/24
2	N	6.11	7/19 (36.8%)	1.35	0/24
All	All	0.83	49/10554 (0.5%)	0.64	0/14269

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	PRO	N-CA	12.87	1.69	1.47
2	K	4	PRO	N-CA	12.32	1.68	1.47
2	J	4	PRO	N-CA	12.26	1.68	1.47
2	H	4	PRO	N-CA	12.26	1.68	1.47
2	I	4	PRO	N-CA	12.00	1.67	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	1464	0	1498	44	0
1	B	1440	0	1474	40	0
1	C	1468	0	1501	56	0
1	D	1468	0	1501	30	0
1	E	1460	0	1497	27	0
1	F	1476	0	1513	49	0
1	G	1460	0	1497	35	0
2	H	56	0	53	8	0
2	I	56	0	53	8	0
2	J	56	0	54	6	0
2	K	56	0	53	6	0
2	L	56	0	53	6	0
2	M	56	0	54	5	0
2	N	56	0	54	8	0
3	A	19	0	0	0	0
3	B	22	0	0	5	0
3	C	22	0	0	0	0
3	D	35	0	0	1	0
3	E	38	0	0	3	0
3	F	38	0	0	1	0
3	G	30	0	0	3	0
3	I	2	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
All	All	10836	0	10855	293	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 14.

The worst 5 of 293 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:F:110:GLY:O	1:F:111:ARG:HG2	1.22	1.33
2:J:4:PRO:N	2:J:4:PRO:CA	1.68	1.32
2:L:4:PRO:CA	2:L:4:PRO:N	1.69	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:PRO:N	2:N:4:PRO:CA	1.67	1.29
2:M:4:PRO:N	2:M:4:PRO:CA	1.67	1.27

There are no symmetry-related clashes.

## 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	185/221 (84%)	171 (92%)	12 (6%)	2 (1%)	14	41
1	B	181/221 (82%)	166 (92%)	12 (7%)	3 (2%)	9	29
1	C	185/221 (84%)	168 (91%)	8 (4%)	9 (5%)	2	7
1	D	185/221 (84%)	175 (95%)	6 (3%)	4 (2%)	6	22
1	E	184/221 (83%)	174 (95%)	6 (3%)	4 (2%)	6	22
1	F	187/221 (85%)	181 (97%)	5 (3%)	1 (0%)	29	61
1	G	184/221 (83%)	177 (96%)	7 (4%)	0	100	100
All	All	1291/1547 (84%)	1212 (94%)	56 (4%)	23 (2%)	8	28

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	C	236	ILE
1	C	293	GLN
1	D	113	GLU
1	D	236	ILE

### 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	162/185 (88%)	155 (96%)	7 (4%)	29	62
1	B	160/185 (86%)	151 (94%)	9 (6%)	21	51
1	C	163/185 (88%)	153 (94%)	10 (6%)	18	48
1	D	163/185 (88%)	155 (95%)	8 (5%)	25	57
1	E	162/185 (88%)	157 (97%)	5 (3%)	40	74
1	F	164/185 (89%)	156 (95%)	8 (5%)	25	57
1	G	162/185 (88%)	154 (95%)	8 (5%)	25	57
2	H	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	2 (100%)	0	100	100
2	N	2/2 (100%)	2 (100%)	0	100	100
All	All	1150/1309 (88%)	1095 (95%)	55 (5%)	25	58

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	221	HIS
1	D	196	SER
1	G	111	ARG
1	C	242	MET
1	D	116	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	237	GLN

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Mol	Chain	Res	Type
1	F	261	GLN
1	G	154	ASN
1	E	237	GLN
1	G	108	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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	WFP	K	2	2	12,13,14	1.11	2 (16%)	14,17,19	1.36	4 (28%)
2	ALO	L	3	2	5,6,7	0.58	0	6,7,9	1.08	1 (16%)
2	ALO	I	3	2	5,6,7	0.41	0	6,7,9	0.45	0
2	ALO	N	3	2	5,6,7	0.41	0	6,7,9	1.67	2 (33%)
2	ALO	K	3	2	5,6,7	0.52	0	6,7,9	1.38	1 (16%)
2	ALO	H	3	2	5,6,7	0.44	0	6,7,9	0.79	0
2	WFP	M	2	2	12,13,14	1.00	1 (8%)	14,17,19	1.66	4 (28%)
2	ALO	J	3	2	5,6,7	0.43	0	6,7,9	1.65	1 (16%)
2	WFP	I	2	2	12,13,14	1.14	1 (8%)	14,17,19	1.85	6 (42%)
2	WFP	N	2	2	12,13,14	1.04	1 (8%)	14,17,19	1.77	4 (28%)
2	WFP	L	2	2	12,13,14	0.98	1 (8%)	14,17,19	2.12	6 (42%)
2	WFP	J	2	2	12,13,14	0.99	1 (8%)	14,17,19	1.48	3 (21%)
2	WFP	H	2	2	12,13,14	0.99	1 (8%)	14,17,19	1.81	4 (28%)
2	ALO	M	3	2	5,6,7	0.38	0	6,7,9	1.27	1 (16%)

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	WFP	K	2	2	-	1/5/6/8	0/1/1/1
2	ALO	L	3	2	-	1/5/6/8	-
2	ALO	I	3	2	-	1/5/6/8	-
2	ALO	N	3	2	-	1/5/6/8	-
2	ALO	K	3	2	-	1/5/6/8	-
2	ALO	H	3	2	-	1/5/6/8	-
2	WFP	M	2	2	-	2/5/6/8	0/1/1/1
2	ALO	J	3	2	-	0/5/6/8	-
2	WFP	I	2	2	-	1/5/6/8	0/1/1/1
2	WFP	N	2	2	-	2/5/6/8	0/1/1/1
2	WFP	L	2	2	-	0/5/6/8	0/1/1/1
2	WFP	J	2	2	-	1/5/6/8	0/1/1/1
2	WFP	H	2	2	-	0/5/6/8	0/1/1/1
2	ALO	M	3	2	-	1/5/6/8	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	WFP	CB-CG	2.49	1.57	1.51
2	M	2	WFP	CB-CG	2.48	1.57	1.51
2	J	2	WFP	CB-CG	2.42	1.57	1.51
2	L	2	WFP	CB-CG	2.34	1.56	1.51
2	N	2	WFP	CB-CG	2.30	1.56	1.51

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	WFP	CG-CB-CA	-3.72	106.57	114.10
2	I	2	WFP	CD2-CE2-CZ	-3.60	118.97	123.52
2	L	2	WFP	CD2-CE2-CZ	-3.53	119.06	123.52
2	H	2	WFP	CD1-CE1-CZ	-3.49	119.11	123.52
2	L	2	WFP	CE2-CZ-CE1	3.38	121.39	116.13

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	3	ALO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	K	3	ALO	O-C-CA-CB
2	M	3	ALO	O-C-CA-CB
2	K	2	WFP	N-CA-CB-CG
2	N	2	WFP	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	ALO	3	0
2	I	3	ALO	4	0
2	N	3	ALO	4	0
2	K	3	ALO	4	0
2	H	3	ALO	2	0
2	J	3	ALO	2	0
2	H	2	WFP	2	0
2	M	3	ALO	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 ⓘ

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	189/221 (85%)	-0.05	10 (5%) 26 17	51, 64, 101, 137	0
1	B	185/221 (83%)	-0.17	7 (3%) 40 30	51, 67, 99, 132	0
1	C	189/221 (85%)	-0.11	14 (7%) 14 8	47, 64, 100, 145	0
1	D	189/221 (85%)	-0.26	8 (4%) 36 26	42, 53, 94, 152	0
1	E	188/221 (85%)	-0.24	5 (2%) 54 44	42, 51, 86, 134	0
1	F	190/221 (85%)	-0.19	12 (6%) 20 12	41, 49, 85, 145	0
1	G	188/221 (85%)	-0.17	13 (6%) 16 10	43, 56, 88, 143	0
2	H	3/7 (42%)	-0.48	0 100 100	72, 72, 72, 75	0
2	I	3/7 (42%)	-0.18	0 100 100	73, 73, 75, 77	0
2	J	3/7 (42%)	-0.39	0 100 100	65, 65, 71, 73	0
2	K	3/7 (42%)	-0.49	0 100 100	62, 62, 64, 68	0
2	L	3/7 (42%)	-0.50	0 100 100	55, 55, 55, 57	0
2	M	3/7 (42%)	-0.46	0 100 100	54, 54, 55, 57	0
2	N	3/7 (42%)	-0.36	0 100 100	52, 52, 55, 56	0
All	All	1339/1596 (83%)	-0.17	69 (5%) 27 18	41, 58, 100, 152	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	THR	9.3
1	G	110	GLY	7.0
1	E	110	GLY	6.0
1	C	294	ASP	5.8
1	D	111	ARG	5.7

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

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALO	K	3	7/8	0.94	0.17	58,62,69,70	0
2	ALO	N	3	7/8	0.95	0.15	44,52,59,61	0
2	ALO	I	3	7/8	0.96	0.14	62,69,73,75	0
2	ALO	H	3	7/8	0.96	0.14	64,66,70,72	0
2	WFP	K	2	13/14	0.97	0.14	54,58,63,65	0
2	ALO	L	3	7/8	0.97	0.12	50,54,56,63	0
2	ALO	J	3	7/8	0.97	0.16	61,67,72,75	0
2	WFP	J	2	13/14	0.97	0.17	55,66,70,70	0
2	WFP	N	2	13/14	0.98	0.15	46,50,54,56	0
2	WFP	L	2	13/14	0.98	0.15	44,49,54,54	0
2	WFP	I	2	13/14	0.98	0.17	63,67,71,71	0
2	WFP	H	2	13/14	0.98	0.13	53,60,69,69	0
2	ALO	M	3	7/8	0.98	0.12	51,53,56,57	0
2	WFP	M	2	13/14	0.99	0.15	45,48,54,55	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.