



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 10:35 pm BST

PDB ID : 3CWU  
Title : Crystal Structure of an AlkA Host/Guest Complex 2'-fluoro-2'-deoxy-1,N6-ethenoadenine:Thymine Base Pair  
Authors : Bowman, B.R.; Lee, S.; Wang, S.; Verdine, G.L.  
Deposited on : 2008-04-22  
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	:	2.11
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)	:	2.11

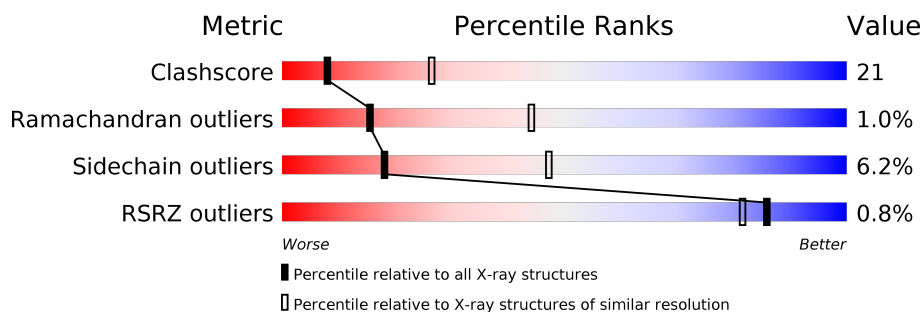
# 1 Overall quality at a glance

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))
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	282	<div> <div style="width: 69%;"></div> <div style="width: 29%;"></div> <div style="width: 2%;"></div> </div>
1	B	282	<div> <div style="width: 61%;"></div> <div style="width: 36%;"></div> <div style="width: 3%;"></div> </div>
1	C	282	<div> <div style="width: 61%;"></div> <div style="width: 35%;"></div> <div style="width: 4%;"></div> </div>
1	D	282	<div> <div style="width: 55%;"></div> <div style="width: 42%;"></div> <div style="width: 3%;"></div> </div>
2	E	12	<div> <div style="width: 50%;"></div> <div style="width: 25%;"></div> <div style="width: 25%;"></div> </div>
2	G	12	<div> <div style="width: 8%;"></div> <div style="width: 67%;"></div> <div style="width: 25%;"></div> </div>
3	F	12	<div> <div style="width: 8%;"></div> <div style="width: 75%;"></div> <div style="width: 17%;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	H	12	

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	2FE	E	8	-	-	X	-
2	2FE	G	8	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9875 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 DNA-3-methyladenine glycosylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	B	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	C	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	D	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(2FE)P\*DTP\*DGP\*DCP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	F	N	O	P	0	0
			247	119	1	48	68	11		
2	G	12	Total	C	F	N	O	P	0	0
			247	119	1	48	68	11		

- Molecule 3 is a DNA chain called DNA (5'-D(\*DGP\*DGP\*DCP\*DAP\*DTP\*DTP\*DCP\*DAP\*DTP\*DGP\*DTP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			242	117	42	72	11			
3	H	12	Total	C	N	O	P	0	0	0
			242	117	42	72	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		

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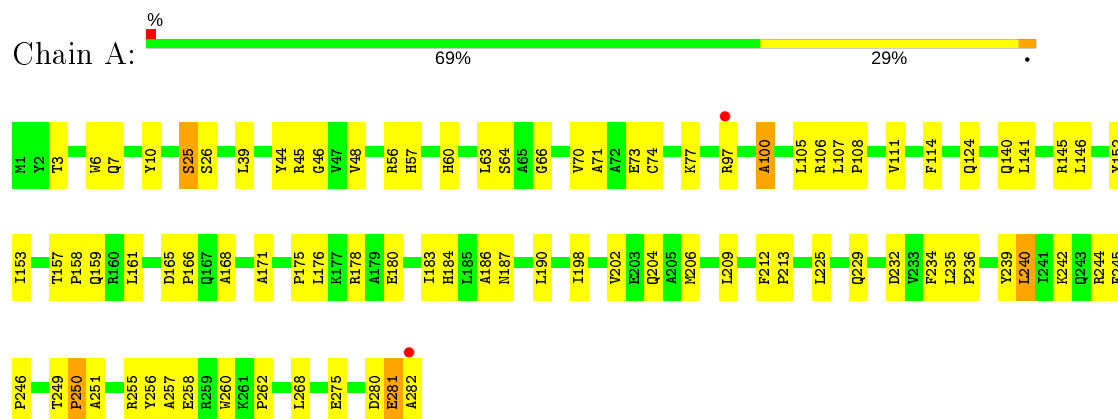
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	11	Total 11	O 11	0	0
4	C	9	Total 9	O 9	0	0
4	D	8	Total 8	O 8	0	0
4	G	1	Total 1	O 1	0	0

### 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 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.

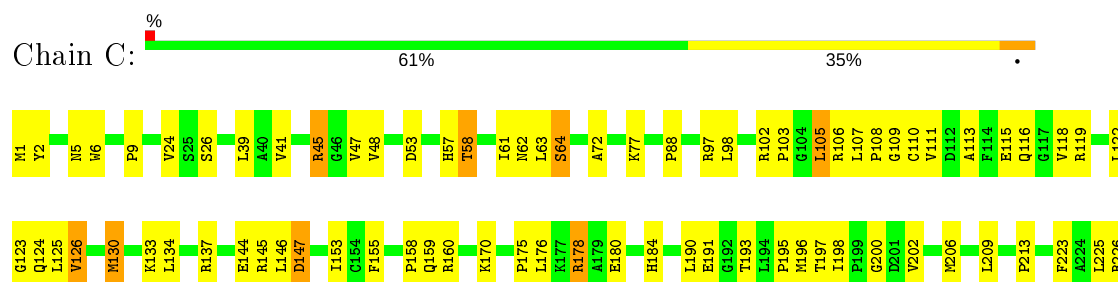
#### • Molecule 1: DNA-3-methyladenine glycosylase 2

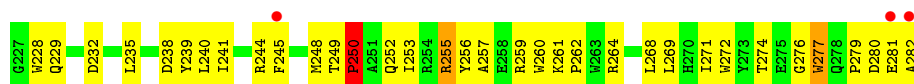


#### • Molecule 1: DNA-3-methyladenine glycosylase 2

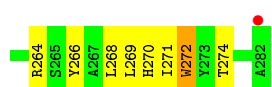
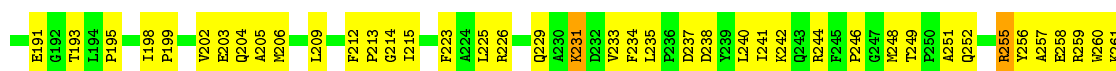


#### • Molecule 1: DNA-3-methyladenine glycosylase 2

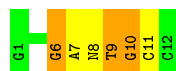




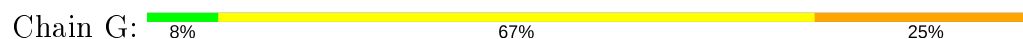
- Molecule 1: DNA-3-methyladenine glycosylase 2



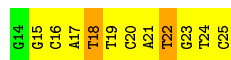
- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(2FE)P\*DTP\*DGP\*DCP\*DC)-3')



- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(2FE)P\*DTP\*DGP\*DCP\*DC)-3')



- Molecule 3: DNA (5'-D(\*DGP\*DGP\*DCP\*DAP\*DTP\*DTP\*DCP\*DAP\*DTP\*DGP\*DTP\*D C)-3')



- Molecule 3: DNA (5'-D(\*DGP\*DGP\*DCP\*DAP\*DTP\*DTP\*DCP\*DAP\*DTP\*DGP\*DTP\*D C)-3')



G14	
A17	
T18	
T19	
C20	
A21	
T22	
G23	
T24	
C25	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.94Å 100.74Å 102.98Å 90.00° 93.86° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 45.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-2.80) 90.9 (45.77-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.273 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: 2FE

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	0.42	0/2277	0.63	0/3104
1	B	0.42	0/2277	0.65	0/3104
1	C	0.43	0/2277	0.65	0/3104
1	D	0.43	0/2277	0.65	1/3104 (0.0%)
2	E	1.05	1/249 (0.4%)	1.27	2/380 (0.5%)
2	G	0.89	0/249	1.23	3/380 (0.8%)
3	F	1.52	5/270 (1.9%)	1.46	2/415 (0.5%)
3	H	0.92	1/270 (0.4%)	1.20	4/415 (1.0%)
All	All	0.54	7/10146 (0.1%)	0.75	12/14006 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	18	DT	C5'-C4'	-8.01	1.42	1.51
3	F	18	DT	N1-C2	6.82	1.43	1.38
3	F	18	DT	C4'-C3'	6.24	1.59	1.53
2	E	6	DG	C5-C6	6.08	1.48	1.42
3	F	19	DT	C5'-C4'	-5.62	1.45	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	10	DG	C5'-C4'-C3'	-6.23	102.88	114.10
2	G	4	DA	C5'-C4'-C3'	-6.18	102.97	114.10
2	E	9	DT	C5'-C4'-C3'	-6.08	103.15	114.10
1	D	105	LEU	CA-CB-CG	6.01	129.13	115.30
3	H	21	DA	C5'-C4'-C3'	-5.92	103.45	114.10

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	2215	0	2209	73	0
1	B	2215	0	2209	99	0
1	C	2215	0	2209	92	0
1	D	2215	0	2209	101	0
2	E	247	0	135	24	0
2	G	247	0	135	20	0
3	F	242	0	138	22	0
3	H	242	0	138	8	0
4	A	8	0	0	0	0
4	B	11	0	0	0	0
4	C	9	0	0	0	0
4	D	8	0	0	0	0
4	G	1	0	0	0	0
All	All	9875	0	9382	411	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 21.

The worst 5 of 411 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)
3:H:21:DA:H2''	3:H:22:DT:H5'	1.20	1.17
2:E:8:2FE:H10	3:F:18:DT:H3	1.14	1.10
1:B:143:GLY:HA3	1:B:153:ILE:HD11	1.35	1.07
2:E:8:2FE:C10	3:F:18:DT:H3	1.70	1.05
1:A:124:GLN:HE21	1:A:178:ARG:HH11	0.97	0.96

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	280/282 (99%)	258 (92%)	18 (6%)	4 (1%)	11	34
1	B	280/282 (99%)	257 (92%)	22 (8%)	1 (0%)	34	66
1	C	280/282 (99%)	260 (93%)	14 (5%)	6 (2%)	7	23
1	D	280/282 (99%)	256 (91%)	24 (9%)	0	100	100
All	All	1120/1128 (99%)	1031 (92%)	78 (7%)	11 (1%)	15	44

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	277	TRP
1	A	281	GLU
1	C	281	GLU
1	A	250	PRO
1	B	275	GLU

### 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	222/222 (100%)	213 (96%)	9 (4%)	30	64
1	B	222/222 (100%)	212 (96%)	10 (4%)	27	60
1	C	222/222 (100%)	207 (93%)	15 (7%)	16	42
1	D	222/222 (100%)	201 (90%)	21 (10%)	8	25
All	All	888/888 (100%)	833 (94%)	55 (6%)	18	47

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

Mol	Chain	Res	Type
1	C	130	MET
1	C	250	PRO

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Mol	Chain	Res	Type
1	D	203	GLU
1	C	144	GLU
1	C	147	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	243	GLN
1	C	159	GLN
1	D	187	ASN
1	C	124	GLN
1	C	221	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	2FE	G	8	2	18,27,28	1.82	3 (16%)	17,40,43	1.92	5 (29%)
2	2FE	E	8	2	18,27,28	2.11	5 (27%)	17,40,43	2.29	7 (41%)

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	2FE	G	8	2	-	2/3/25/26	0/4/4/4
2	2FE	E	8	2	-	2/3/25/26	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	8	2FE	C6-N6	-4.84	1.28	1.33
2	E	8	2FE	C5-C6	-4.66	1.34	1.38
2	G	8	2FE	C5-C6	4.37	1.43	1.38
2	G	8	2FE	C6-N6	-4.30	1.29	1.33
2	E	8	2FE	O5'-C5'	-3.28	1.36	1.44

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	2FE	C2-N3-C4	-5.60	109.58	116.58
2	G	8	2FE	C2-N3-C4	-4.03	111.54	116.58
2	E	8	2FE	C4-C5-N7	3.57	113.12	109.40
2	E	8	2FE	F1'-C2'-C1'	3.29	115.93	109.08
2	G	8	2FE	C2'-C3'-C4'	3.27	106.63	102.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	8	2FE	C4'-C5'-O5'-P
2	G	8	2FE	C3'-C4'-C5'-O5'
2	E	8	2FE	C3'-C4'-C5'-O5'
2	E	8	2FE	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	8	2FE	7	0
2	E	8	2FE	11	0

## 5.5 Carbohydrates

There are no carbohydrates 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 ⓘ

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	282/282 (100%)	-0.15	2 (0%) 87 84	29, 44, 76, 101	0
1	B	282/282 (100%)	-0.31	3 (1%) 80 75	23, 37, 56, 97	0
1	C	282/282 (100%)	-0.28	3 (1%) 80 75	23, 38, 66, 104	0
1	D	282/282 (100%)	-0.21	1 (0%) 92 91	23, 48, 64, 99	0
2	E	11/12 (91%)	-0.03	0 100 100	55, 82, 105, 112	0
2	G	11/12 (91%)	0.10	0 100 100	56, 72, 87, 90	0
3	F	12/12 (100%)	0.09	0 100 100	51, 102, 113, 115	0
3	H	12/12 (100%)	-0.16	0 100 100	38, 64, 93, 94	0
All	All	1174/1176 (99%)	-0.23	9 (0%) 86 81	23, 42, 74, 115	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	4.9
1	D	282	ALA	4.8
1	A	282	ALA	4.1
1	B	282	ALA	3.9
1	C	281	GLU	3.8

### 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	2FE	E	8	24/25	0.87	0.17	78,80,89,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2FE	G	8	24/25	0.93	0.16	59,66,73,77	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.