



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3F07  
Title : Crystal Structure Analysis of Human HDAC8 complexed with APHA in a new monoclinic crystal form  
Authors : Dowling, D.P.; Gantt, S.L.; Gattis, S.G.; Fierke, C.A.; Christianson, D.W.  
Deposited on : 2008-10-24  
Resolution : 3.30 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.

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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

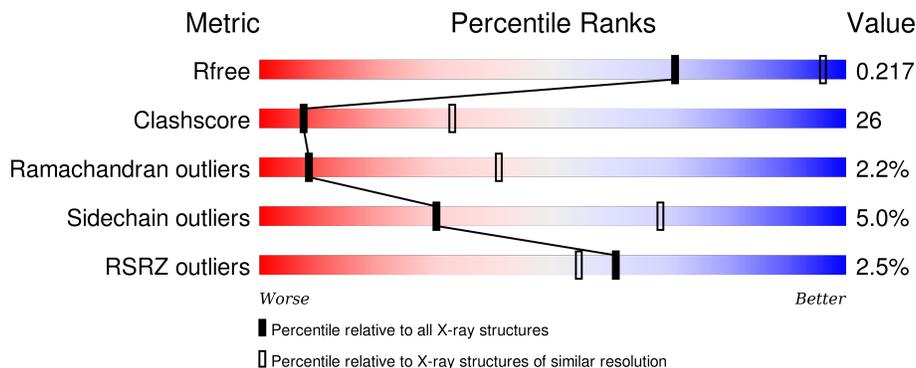
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	388	 4% 54% 35% • 6%
1	B	388	 2% 51% 39% 5% 5%
1	C	388	 4% 50% 33% • 12%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8443 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 Histone deacetylase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	Total 2853	C 1828	N 474	O 532	S 19	0	0	0
1	B	368	Total 2866	C 1835	N 476	O 536	S 19	0	0	0
1	C	340	Total 2658	C 1710	N 445	O 485	S 18	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
A	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
A	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
A	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
A	382	SER	-	EXPRESSION TAG	UNP Q9BY41
A	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
B	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
B	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
B	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
B	382	SER	-	EXPRESSION TAG	UNP Q9BY41
B	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	378	ILE	-	EXPRESSION TAG	UNP Q9BY41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
C	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
C	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
C	382	SER	-	EXPRESSION TAG	UNP Q9BY41
C	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	388	HIS	-	EXPRESSION TAG	UNP Q9BY41

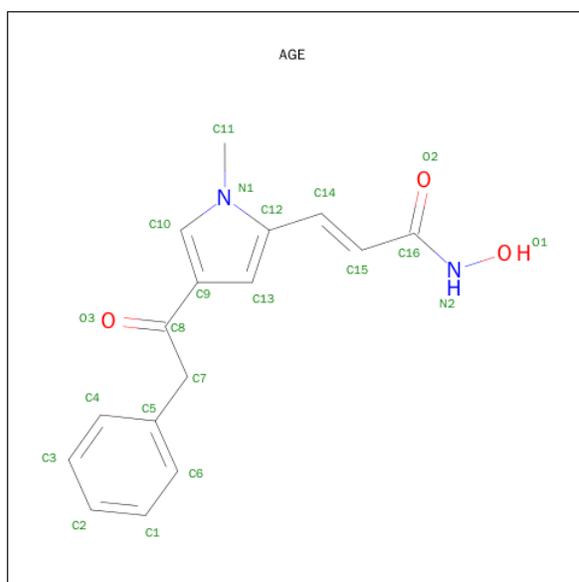
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	2	Total Zn 2 2	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is (2E)-N-HYDROXY-3-[1-METHYL-4-(PHENYLACETYL)-1H-PYRROL-2-YL]PROP-2-ENAMIDE (three-letter code: AGE) (formula: C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>).

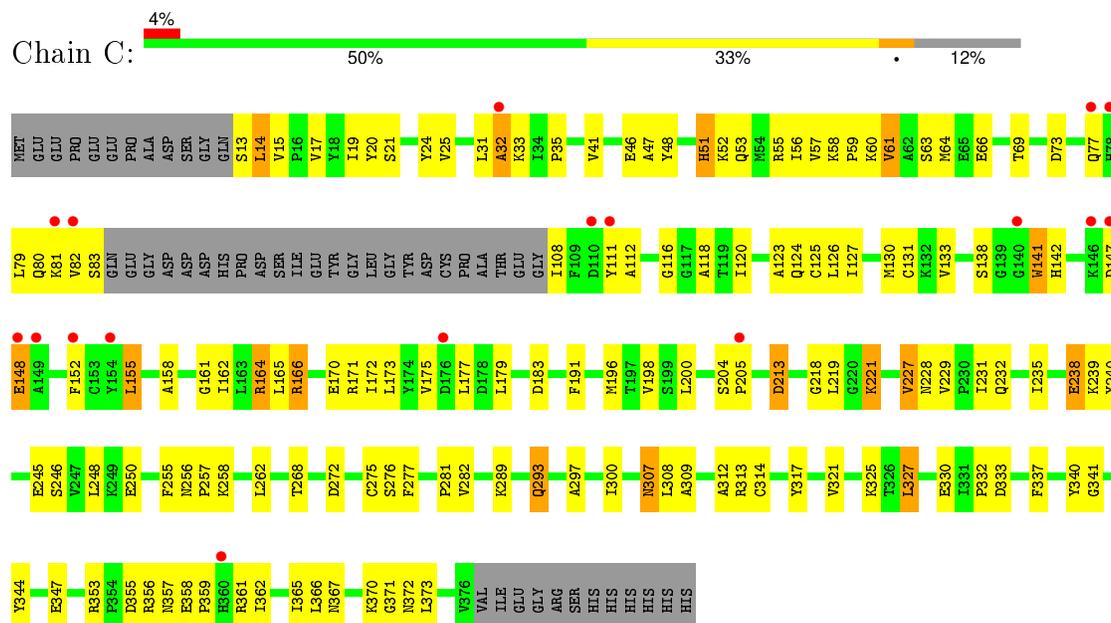


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	N	O	0	0
			21	16	2	3		
4	B	1	Total	C	N	O	0	0
			21	16	2	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	3	Total	O	0	0
			3	3		
5	C	6	Total	O	0	0
			6	6		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.38Å 90.17Å 92.27Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	31.50 – 3.30 31.50 – 3.28	Depositor EDS
% Data completeness (in resolution range)	95.2 (31.50-3.30) 98.0 (31.50-3.28)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.216 , 0.260 0.222 , 0.217	Depositor DCC
$R_{free}$ test set	1107 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.5	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21899 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: K, AGE, ZN

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	0.40	0/2924	0.63	1/3968 (0.0%)
1	B	0.41	0/2937	0.64	1/3985 (0.0%)
1	C	0.44	0/2723	0.64	1/3691 (0.0%)
All	All	0.41	0/8584	0.64	3/11644 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASN	N-CA-C	-6.28	94.04	111.00
1	C	307	ASN	N-CA-C	-5.89	95.09	111.00
1	B	307	ASN	N-CA-C	-5.86	95.19	111.00

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	A	2853	0	2804	139	0
1	B	2866	0	2813	154	0
1	C	2658	0	2642	138	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	21	0	16	3	0
4	B	21	0	16	3	0
5	A	5	0	0	0	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0
All	All	8443	0	8291	427	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 26.

The worst 5 of 427 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:B:13:SER:HB2	1:B:15:VAL:HG12	1.54	0.90
1:A:221:LYS:CE	1:A:221:LYS:H	1.86	0.89
1:C:221:LYS:CE	1:C:221:LYS:H	1.85	0.88
1:B:221:LYS:CE	1:B:221:LYS:H	1.87	0.88
1:A:13:SER:HB2	1:A:15:VAL:HG12	1.55	0.87

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	364/388 (94%)	306 (84%)	51 (14%)	7 (2%)	<b>10</b> 45
1	B	366/388 (94%)	310 (85%)	46 (13%)	10 (3%)	<b>6</b> 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	336/388 (87%)	291 (87%)	39 (12%)	6 (2%)	11	46
All	All	1066/1164 (92%)	907 (85%)	136 (13%)	23 (2%)	8	41

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	148	GLU
1	A	213	ASP
1	B	148	GLU
1	B	213	ASP

### 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	A	307/326 (94%)	290 (94%)	17 (6%)	27	66
1	B	308/326 (94%)	294 (96%)	14 (4%)	34	72
1	C	286/326 (88%)	272 (95%)	14 (5%)	31	69
All	All	901/978 (92%)	856 (95%)	45 (5%)	30	68

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	B	221	LYS
1	C	238	GLU
1	B	142	HIS
1	B	227	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	84	GLN
1	B	236	GLN
1	C	293	GLN
1	B	90	HIS
1	B	253	GLN

### 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](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
4	AGE	A	500	-	19,22,22	3.48	13 (68%)	21,29,29	3.52	6 (28%)
4	AGE	B	501	-	19,22,22	3.04	13 (68%)	21,29,29	2.59	6 (28%)

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
4	AGE	A	500	-	-	2/9/15/15	0/2/2/2
4	AGE	B	501	-	-	2/9/15/15	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	AGE	O1-N2	-4.18	1.32	1.39
4	A	500	AGE	O1-N2	-3.98	1.32	1.39
4	B	501	AGE	C10-N1	-2.06	1.35	1.38
4	B	501	AGE	C15-C14	2.05	1.38	1.32
4	B	501	AGE	C15-C16	2.11	1.52	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	AGE	C7-C5-C4	-4.53	114.07	120.86
4	B	501	AGE	C7-C5-C4	-4.13	114.66	120.86
4	A	500	AGE	O3-C8-C9	-3.72	114.69	120.71
4	A	500	AGE	C11-N1-C10	-2.83	120.29	125.04
4	B	501	AGE	C11-N1-C10	-2.73	120.45	125.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	AGE	O3-C8-C7-C5
4	A	500	AGE	O3-C8-C7-C5
4	B	501	AGE	C9-C8-C7-C5
4	A	500	AGE	C9-C8-C7-C5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	AGE	3	0
4	B	501	AGE	3	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	366/388 (94%)	-0.11	2 (0%) 91 90	36, 59, 78, 96	0
1	B	368/388 (94%)	-0.11	8 (2%) 65 59	34, 59, 82, 106	0
1	C	340/388 (87%)	0.06	17 (5%) 32 26	39, 61, 78, 86	0
All	All	1074/1164 (92%)	-0.06	27 (2%) 61 54	34, 59, 79, 106	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	ALA	3.6
1	C	81	LYS	3.6
1	C	78	HIS	3.3
1	C	148	GLU	3.1
1	C	77	GLN	3.1

### 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( $\text{\AA}^2$ )	Q<0.9
4	AGE	A	500	21/21	0.88	0.34	1.44	59,66,69,70	21
3	K	B	405	1/1	0.98	0.23	1.21	47,47,47,47	0
4	AGE	B	501	21/21	0.90	0.36	0.95	67,72,76,76	21
3	K	C	407	1/1	0.95	0.32	0.84	38,38,38,38	0
3	K	A	401	1/1	0.97	0.29	0.60	35,35,35,35	0
3	K	B	404	1/1	0.94	0.20	-0.39	35,35,35,35	0
3	K	C	408	1/1	0.95	0.12	-1.25	51,51,51,51	0
3	K	A	402	1/1	0.96	0.12	-1.55	45,45,45,45	0
2	ZN	A	400	1/1	1.00	0.15	-1.73	37,37,37,37	0
2	ZN	C	406	1/1	0.98	0.14	-1.86	48,48,48,48	0
2	ZN	A	409	1/1	0.94	0.05	-1.99	68,68,68,68	1
2	ZN	B	403	1/1	0.98	0.14	-2.01	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.