



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:09 am GMT

PDB ID : 3A6F  
Title : W174F mutant creatininase, Type II  
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.  
Deposited on : 2009-08-31  
Resolution : 1.78 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 : 1.7.2 (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

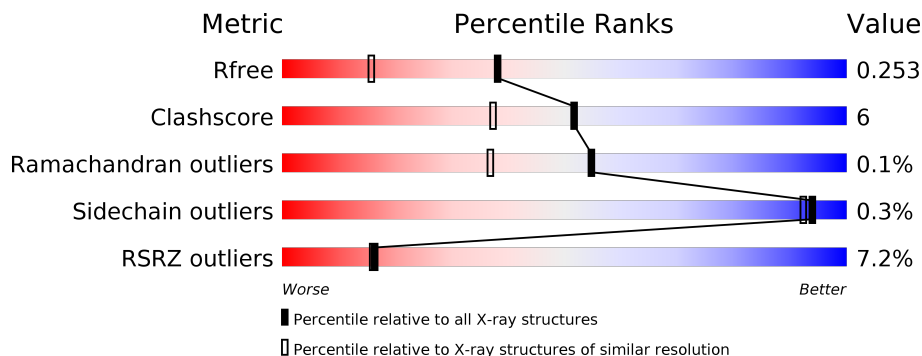
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	260	<div> <div>8%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	B	260	<div> <div>9%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	260	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	D	260	<div> <div>8%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	E	260	<div> <div>6%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	F	260	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12656 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 Creatinine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1984	1271	337	365	11			
1	B	257	Total	C	N	O	S	0	0	0
			1981	1269	336	365	11			
1	C	257	Total	C	N	O	S	0	0	0
			1977	1267	335	364	11			
1	D	257	Total	C	N	O	S	0	0	0
			1977	1266	335	365	11			
1	E	257	Total	C	N	O	S	0	0	0
			1970	1263	334	362	11			
1	F	256	Total	C	N	O	S	0	0	0
			1961	1257	332	361	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	PHE	TRP	ENGINEERED	UNP P83772
B	174	PHE	TRP	ENGINEERED	UNP P83772
C	174	PHE	TRP	ENGINEERED	UNP P83772
D	174	PHE	TRP	ENGINEERED	UNP P83772
E	174	PHE	TRP	ENGINEERED	UNP P83772
F	174	PHE	TRP	ENGINEERED	UNP P83772

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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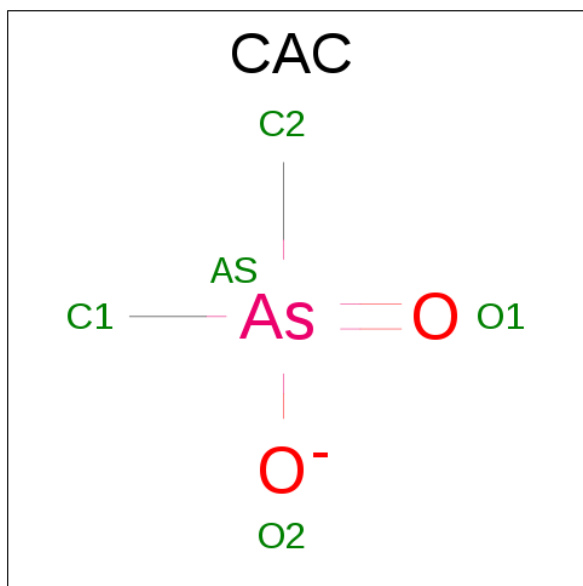
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		
4	E	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		

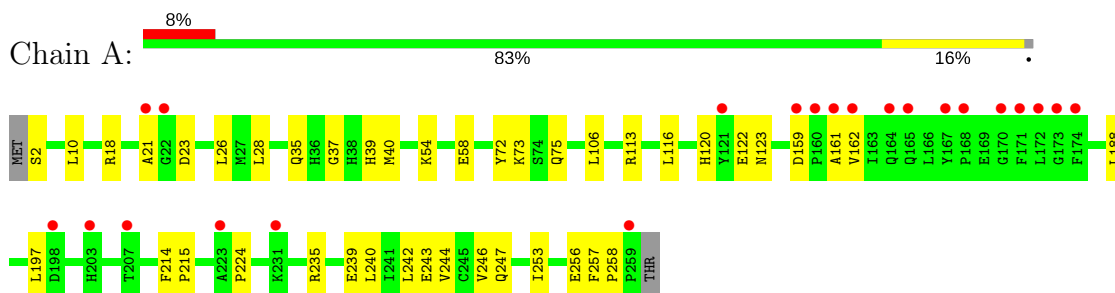
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	124	Total	O	0	0
			124	124		
5	C	126	Total	O	0	0
			126	126		
5	D	128	Total	O	0	0
			128	128		
5	E	125	Total	O	0	0
			125	125		
5	F	150	Total	O	0	0
			150	150		

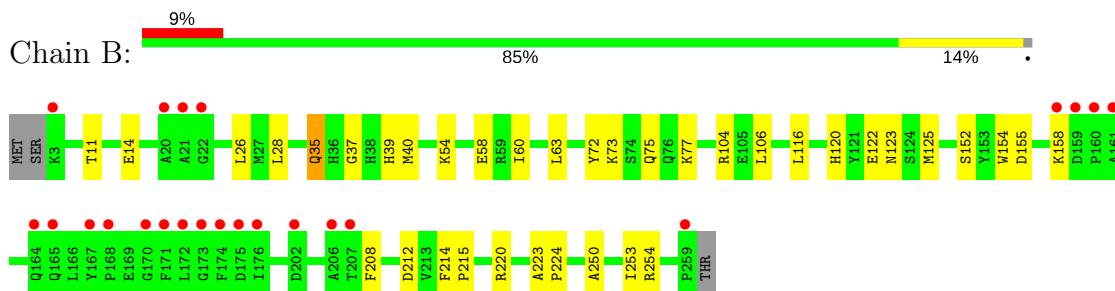
### 3 Residue-property plots

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.

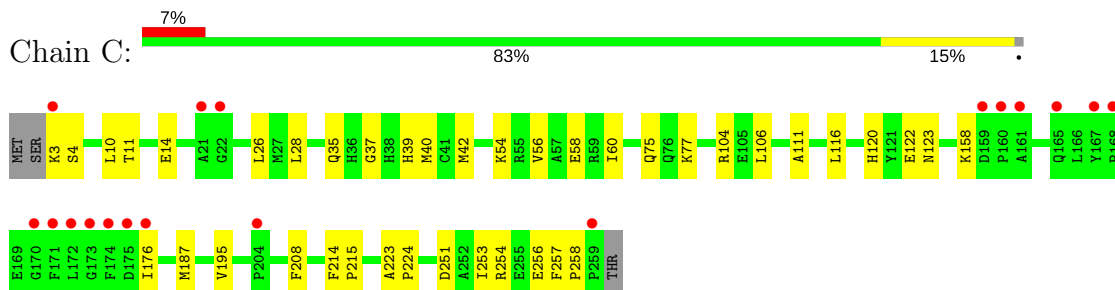
- Molecule 1: Creatinine amidohydrolase



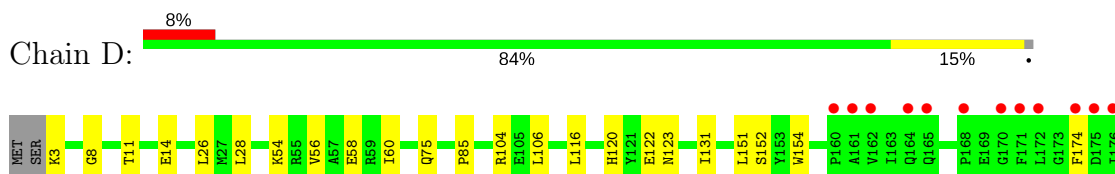
- Molecule 1: Creatinine amidohydrolase

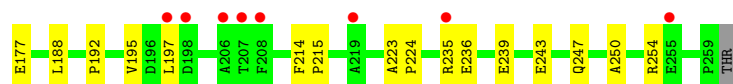


- Molecule 1: Creatinine amidohydrolase

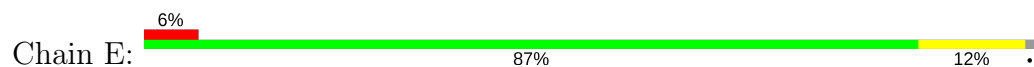


- Molecule 1: Creatinine amidohydrolase

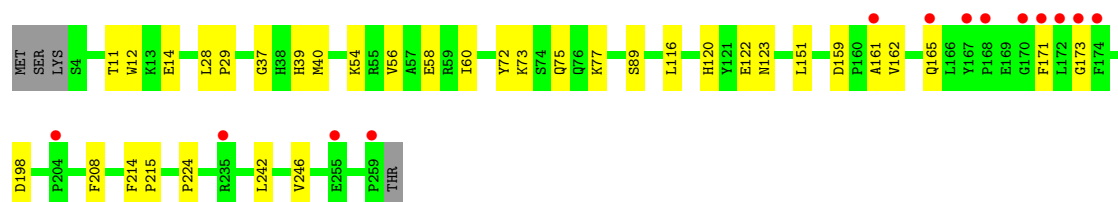
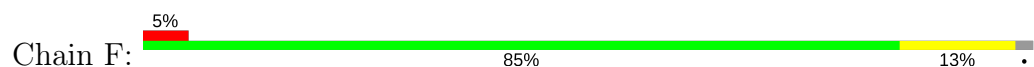




• Molecule 1: Creatinine amidohydrolase



• Molecule 1: Creatinine amidohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.30Å 164.30Å 163.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.78 32.59 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.78) 99.8 (32.59-1.78)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.257 0.233 , 0.253	Depositor DCC
$R_{free}$ test set	12157 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: CAC, ZN, MN

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	0.32	0/2032	0.57	0/2764
1	B	0.32	0/2029	0.58	0/2760
1	C	0.33	0/2025	0.57	0/2755
1	D	0.33	0/2025	0.57	0/2756
1	E	0.34	0/2018	0.58	0/2747
1	F	0.33	0/2009	0.58	0/2736
All	All	0.33	0/12138	0.58	0/16518

There are no bond length outliers.

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	1984	0	1967	27	0
1	B	1981	0	1964	26	0
1	C	1977	0	1958	27	0
1	D	1977	0	1953	30	0
1	E	1970	0	1945	23	0
1	F	1961	0	1932	21	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
5	A	111	0	0	1	0
5	B	124	0	0	3	0
5	C	126	0	0	3	0
5	D	128	0	0	4	0
5	E	125	0	0	2	0
5	F	150	0	0	1	0
All	All	12656	0	11719	152	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 6.

The worst 5 of 152 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:E:120:HIS:HB3	1:E:123:ASN:ND2	1.94	0.81
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.00	0.76
1:C:28:LEU:HD23	1:C:116:LEU:HD21	1.69	0.75
1:A:54:LYS:O	1:A:58:GLU:HG3	1.90	0.72
1:D:188:LEU:O	1:D:192:PRO:HG3	1.91	0.70

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	256/260 (98%)	247 (96%)	9 (4%)	0	100	100
1	B	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	C	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	D	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	E	255/260 (98%)	248 (97%)	6 (2%)	1 (0%)	38	21
1	F	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
All	All	1530/1560 (98%)	1488 (97%)	41 (3%)	1 (0%)	55	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	124	SER

### 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	211/215 (98%)	211 (100%)	0	100	100
1	B	211/215 (98%)	209 (99%)	2 (1%)	82	76
1	C	210/215 (98%)	209 (100%)	1 (0%)	91	89
1	D	210/215 (98%)	210 (100%)	0	100	100
1	E	208/215 (97%)	207 (100%)	1 (0%)	91	89
1	F	207/215 (96%)	207 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1257/1290 (97%)	1253 (100%)	4 (0%)	94 92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	212	ASP
1	C	158	LYS
1	E	212	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	F	120	HIS
1	D	247	GLN
1	A	165	GLN
1	B	123	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	CAC	A	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	C	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	D	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	E	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	F	303	3,2	0,4,4	0.00	-	0,6,6	0.00	-

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	CAC	A	303	3,2	-	0/0/0/0	0/0/0/0
4	CAC	B	303	3,2	-	0/0/0/0	0/0/0/0
4	CAC	C	303	3,2	-	0/0/0/0	0/0/0/0
4	CAC	D	303	3,2	-	0/0/0/0	0/0/0/0
4	CAC	E	303	3,2	-	0/0/0/0	0/0/0/0
4	CAC	F	303	3,2	-	0/0/0/0	0/0/0/0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	CAC	1	0
4	B	303	CAC	1	0
4	C	303	CAC	1	0
4	E	303	CAC	1	0

## 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 [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	258/260 (99%)	0.43	22 (8%)	11 11	12, 24, 47, 59	0
1	B	257/260 (98%)	0.35	23 (8%)	10 10	14, 22, 43, 56	0
1	C	257/260 (98%)	0.42	18 (7%)	17 17	13, 23, 44, 54	0
1	D	257/260 (98%)	0.33	20 (7%)	14 14	12, 23, 43, 53	0
1	E	257/260 (98%)	0.37	15 (5%)	24 23	11, 21, 41, 56	0
1	F	256/260 (98%)	0.30	13 (5%)	29 28	12, 20, 41, 58	0
All	All	1542/1560 (98%)	0.37	111 (7%)	16 16	11, 22, 44, 59	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	9.0
1	F	172	LEU	8.9
1	F	171	PHE	8.6
1	A	171	PHE	8.3
1	D	171	PHE	7.9

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CAC	B	303	5/5	0.98	0.13	1.80	30,30,35,35	0
4	CAC	A	303	5/5	0.96	0.14	1.54	38,38,40,40	0
4	CAC	E	303	5/5	0.97	0.12	1.48	34,34,36,37	0
4	CAC	C	303	5/5	0.98	0.11	0.10	35,37,38,39	0
2	MN	F	300	1/1	0.94	0.10	-0.05	36,36,36,36	0
4	CAC	F	303	5/5	0.98	0.09	-0.44	26,30,32,34	0
4	CAC	D	303	5/5	0.98	0.09	-0.52	32,33,35,36	0
2	MN	B	300	1/1	0.97	0.08	-0.62	39,39,39,39	0
2	MN	D	300	1/1	0.98	0.09	-0.85	40,40,40,40	0
2	MN	A	300	1/1	0.99	0.03	-2.80	34,34,34,34	0
2	MN	E	300	1/1	0.99	0.05	-3.14	33,33,33,33	0
3	ZN	F	301	1/1	1.00	0.04	-3.23	24,24,24,24	0
3	ZN	C	301	1/1	1.00	0.05	-3.31	25,25,25,25	0
3	ZN	B	301	1/1	0.99	0.04	-3.63	26,26,26,26	0
2	MN	C	300	1/1	0.99	0.04	-3.84	31,31,31,31	0
3	ZN	A	301	1/1	0.99	0.03	-4.39	27,27,27,27	0
3	ZN	E	301	1/1	0.99	0.02	-6.20	25,25,25,25	0
3	ZN	D	301	1/1	0.99	0.04	-7.29	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.