



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:33 am GMT

PDB ID : 4XZ3  
Title : Ca. Korarchaeum cryptofilum dinucleotide forming Acetyl-coenzyme A synthetase 1 (Se-Met derivative) in complex with coenzyme A and Mg-AMPPCP, phosphohistidine segment pointing towards nucleotide binding site  
Authors : Weisse, R.H.-J.; Scheidig, A.J.  
Deposited on : 2015-02-03  
Resolution : 2.40 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

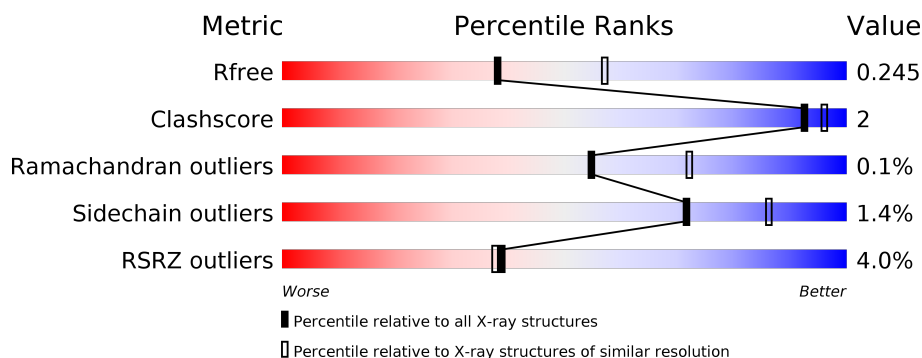
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	464	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	C	464	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>3%</div> </div> </div>
2	B	230	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
2	D	230	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	A	503	-	-	-	X
5	MG	C	502	-	-	-	X
5	MG	C	503	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21079 atoms, of which 10529 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 Acyl-CoA synthetase (NDP forming).

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	463	Total	C	H	N	O	S	Se		0	0	0
			6940	2205	3492	574	655	3	11				
1	C	461	Total	C	H	N	O	S	Se		0	0	0
			6912	2198	3476	570	654	3	11				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP B1L3C9
C	1	MSE	-	initiating methionine	UNP B1L3C9

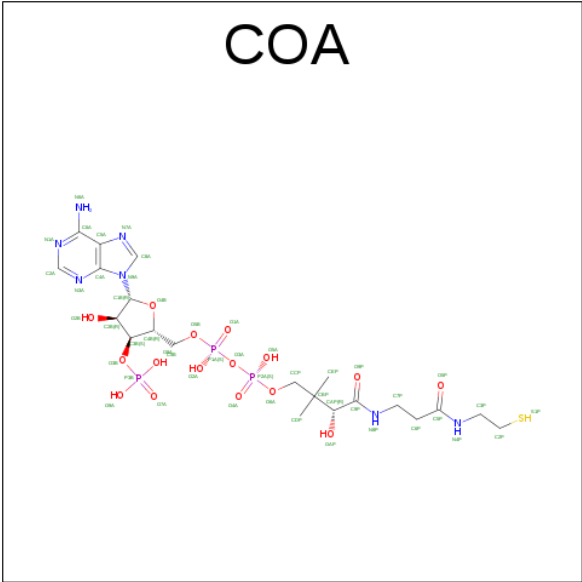
- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
2	B	228	Total	C	H	N	O	Se			0	1	0
			3631	1145	1841	307	334	4					
2	D	213	Total	C	H	N	O	Se			0	0	0
			3225	1038	1612	276	295	4					

There are 2 discrepancies between the modelled and reference sequences:

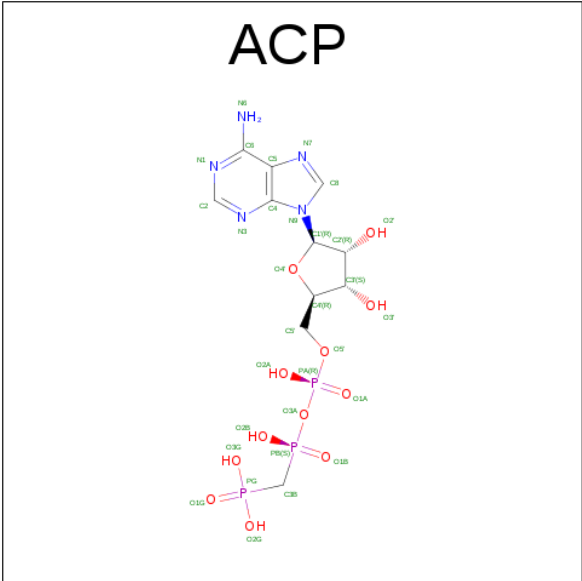
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP B1L7P8
D	1	MSE	-	initiating methionine	UNP B1L7P8

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			80	21	32	7	16	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			80	21	32	7	16	3	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P		0	0
			31	6	9	1	12	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	
			44	11	13	5	12	3	
4	C	1	Total	C	H	N	O	P	
			31	6	9	1	12	3	
4	D	1	Total	C	H	N	O	P	
			44	11	13	5	12	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg		
			1	1	0	0
5	A	1	Total	Mg		
			1	1	0	0
5	D	1	Total	Mg		
			1	1	0	0
5	C	2	Total	Mg		
			2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O		
			23	23	0	0
6	B	11	Total	O		
			11	11	0	0
6	C	21	Total	O		
			21	21	0	0
6	D	1	Total	O		
			1	1	0	0

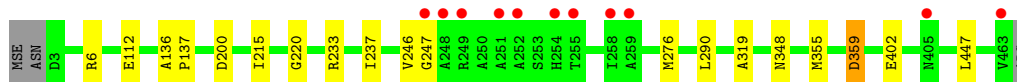
### 3 Residue-property plots [i](#)

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.

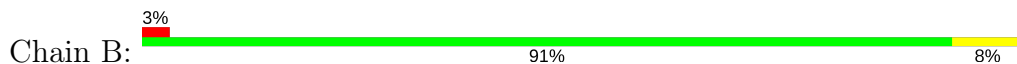
- Molecule 1: Acyl-CoA synthetase (NDP forming)



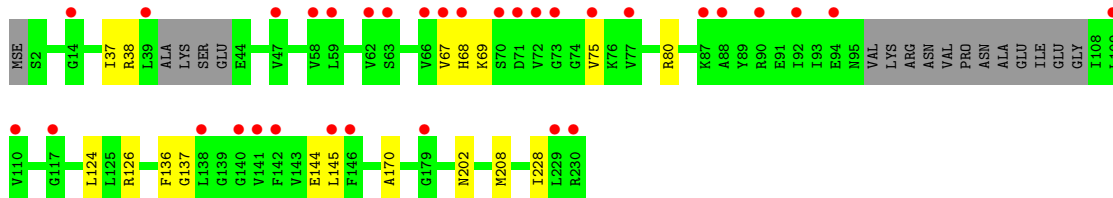
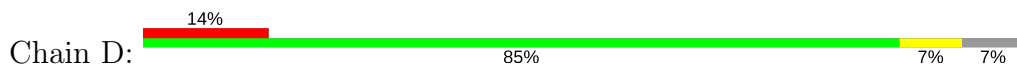
- Molecule 1: Acyl-CoA synthetase (NDP forming)



- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.17Å 111.88Å 127.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 2.40 48.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.84-2.40) 99.8 (48.84-2.40)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.197 , 0.244 0.198 , 0.245	Depositor DCC
$R_{free}$ test set	2877 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MG, ACP

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	0.25	0/3505	0.40	0/4743
1	C	0.25	0/3493	0.40	0/4729
2	B	0.25	0/1817	0.44	0/2445
2	D	0.25	0/1634	0.44	0/2202
All	All	0.25	0/10449	0.41	0/14119

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 [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	3448	3492	3494	12	0
1	C	3436	3476	3478	8	0
2	B	1790	1841	1843	11	0
2	D	1613	1612	1614	11	0
3	A	48	32	32	1	0
3	C	48	32	32	0	0
4	A	22	9	10	1	0
4	B	31	13	14	1	0
4	C	22	9	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	13	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	0	0	0
6	B	11	0	0	0	0
6	C	21	0	0	0	0
6	D	1	0	0	0	0
All	All	10550	10529	10541	38	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 2.

The worst 5 of 38 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:A:113:GLU:OE2	1:A:116:ARG:NH1	2.36	0.58
2:B:173:LEU:HG	2:D:145:LEU:HD11	1.88	0.55
1:A:187:LYS:NZ	1:A:192:ASP:OD1	2.31	0.51
1:C:359:ASP:OD2	1:C:359:ASP:N	2.32	0.50
2:B:51:ARG:NH2	2:B:82:GLU:OE1	2.45	0.49

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	461/464 (99%)	446 (97%)	14 (3%)	1 (0%)	51 67
1	C	459/464 (99%)	441 (96%)	17 (4%)	1 (0%)	51 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	227/230 (99%)	220 (97%)	7 (3%)	0	100	100
2	D	207/230 (90%)	201 (97%)	6 (3%)	0	100	100
All	All	1354/1388 (98%)	1308 (97%)	44 (3%)	2 (0%)	55	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	C	348	ASN

### 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	366/358 (102%)	360 (98%)	6 (2%)	68	83
1	C	365/358 (102%)	359 (98%)	6 (2%)	68	83
2	B	194/192 (101%)	192 (99%)	2 (1%)	80	91
2	D	165/192 (86%)	164 (99%)	1 (1%)	89	95
All	All	1090/1100 (99%)	1075 (99%)	15 (1%)	71	86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	146	PHE
2	B	169	LYS
1	C	359	ASP
1	A	355	MSE
1	C	355	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 11 ligands modelled in this entry, 5 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$
3	COA	A	501	-	43,50,50	0.50	0	48,75,75	0.55	0
4	ACP	A	502	5	18,22,33	0.82	2 (11%)	24,35,52	1.22	3 (12%)
4	ACP	B	300	5	27,33,33	0.86	2 (7%)	30,52,52	1.14	3 (10%)
4	ACP	C	501	5	18,22,33	1.00	2 (11%)	24,35,52	1.15	3 (12%)
3	COA	C	504	-	43,50,50	0.44	0	48,75,75	0.54	0
4	ACP	D	300	5	27,33,33	0.95	2 (7%)	30,52,52	1.04	3 (10%)

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
3	COA	A	501	-	-	0/44/64/64	0/3/3/3
4	ACP	A	502	5	-	0/15/34/38	0/1/1/3
4	ACP	B	300	5	-	0/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	C	501	5	-	0/15/34/38	0/1/1/3
3	COA	C	504	-	-	0/44/64/64	0/3/3/3
4	ACP	D	300	5	-	0/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	ACP	PG-O2G	-2.13	1.49	1.54
4	B	300	ACP	PG-O3G	-2.08	1.50	1.54
4	C	501	ACP	PG-O3G	-2.07	1.50	1.54
4	A	502	ACP	PG-O2G	-2.07	1.50	1.54
4	A	502	ACP	PG-O1G	2.14	1.54	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	300	ACP	O1G-PG-C3B	-2.42	105.87	111.22
4	C	501	ACP	O1G-PG-C3B	-2.36	106.02	111.22
4	A	502	ACP	O1G-PG-C3B	-2.33	106.07	111.22
4	D	300	ACP	O1G-PG-C3B	-2.32	106.10	111.22
4	A	502	ACP	O2G-PG-C3B	2.34	112.07	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	COA	1	0
4	A	502	ACP	1	0
4	B	300	ACP	1	0

## 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 [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	452/464 (97%)	0.23	3 (0%) 87 86	29, 47, 81, 110	0
1	C	450/464 (96%)	0.28	11 (2%) 59 56	29, 47, 81, 124	0
2	B	224/230 (97%)	0.30	6 (2%) 55 52	34, 63, 97, 118	0
2	D	209/230 (90%)	0.92	33 (15%) 2 2	37, 79, 136, 165	0
All	All	1335/1388 (96%)	0.37	53 (3%) 39 38	29, 53, 105, 165	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	VAL	6.5
2	D	140	GLY	6.0
1	C	255	THR	6.0
2	D	62	VAL	5.4
2	D	71	ASP	4.9

### 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
5	MG	C	503	1/1	0.91	0.29	6.72	59,59,59,59	0
5	MG	A	503	1/1	0.69	0.22	6.66	57,57,57,57	0
5	MG	C	502	1/1	0.92	0.27	3.96	62,62,62,62	0
4	ACP	A	502	22/31	0.90	0.17	0.28	63,91,115,123	0
4	ACP	D	300	31/31	0.81	0.23	-0.25	91,134,166,177	0
3	COA	A	501	48/48	0.93	0.14	-0.53	52,69,81,93	0
3	COA	C	504	48/48	0.95	0.13	-0.80	46,64,79,84	0
4	ACP	C	501	22/31	0.92	0.11	-0.96	53,82,107,115	0
4	ACP	B	300	31/31	0.96	0.12	-1.16	51,69,85,90	0
5	MG	B	301	1/1	0.84	0.11	-	57,57,57,57	0
5	MG	D	301	1/1	0.81	0.08	-	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.