



# wwPDB X-ray Structure Validation Summary Report

Feb 15, 2017 – 02:41 am GMT

PDB ID : 2NRB  
Title : C28S Mutant of Succinyl-CoA:3-Ketoacid CoA Transferase from Pig Heart  
Authors : Tammam, S.D.; Fraser, M.E.  
Deposited on : 2006-11-01  
Resolution : 2.00 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  
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

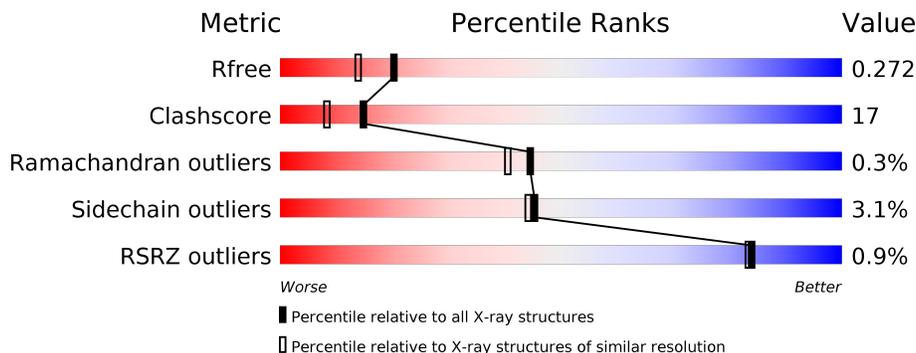
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	481	 % 65% 30% ..
1	B	481	 % 67% 28% ..
1	C	481	 % 65% 31% ..
1	D	481	 % 61% 34% ..

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 15104 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3561	2260	611	673	17	0	0	0
1	B	470	3582	2271	614	680	17	0	0	0
1	C	467	3561	2260	611	673	17	0	0	0
1	D	469	3578	2269	613	679	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	CYS	ENGINEERED	UNP Q29551
B	28	SER	CYS	ENGINEERED	UNP Q29551
C	28	SER	CYS	ENGINEERED	UNP Q29551
D	28	SER	CYS	ENGINEERED	UNP Q29551

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	217	Total	O	0	0
			217	217		
3	C	242	Total	O	0	0
			242	242		

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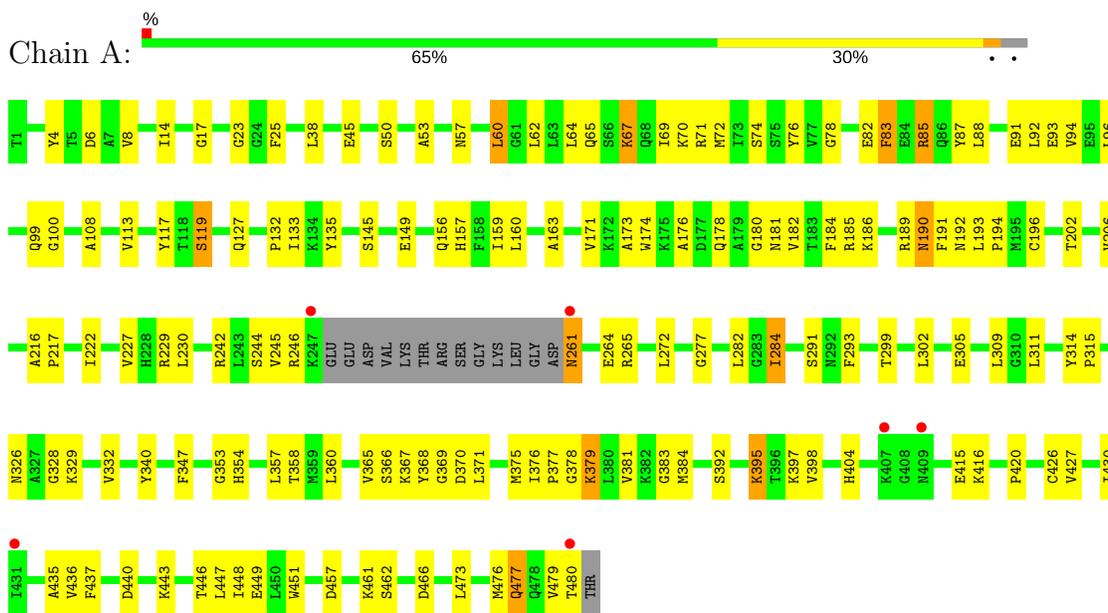
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	D	193	Total 193	O 193	0	0

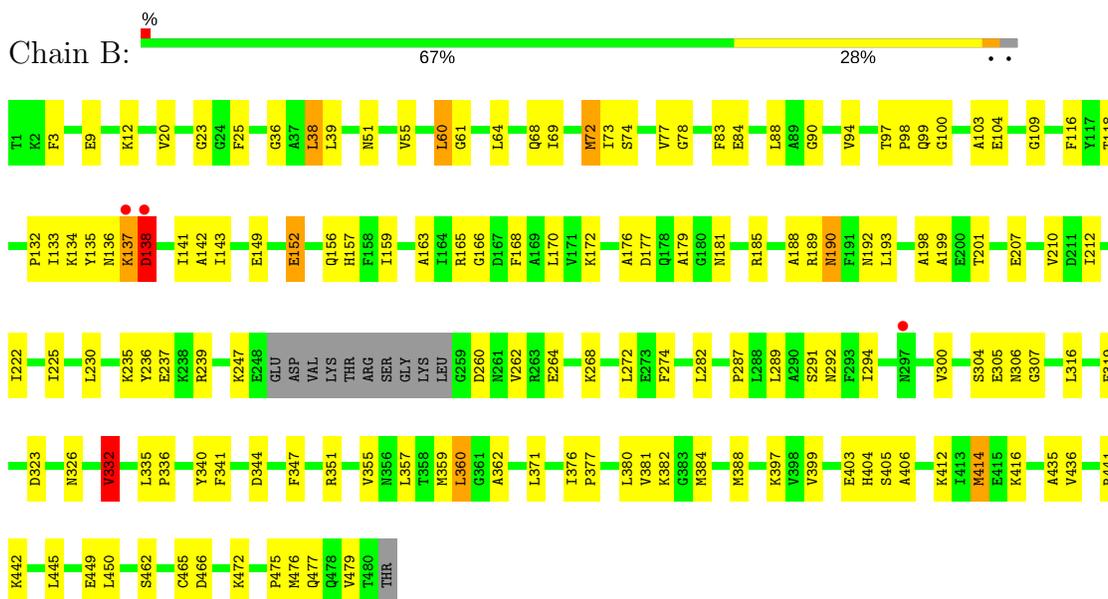
### 3 Residue-property plots [i](#)

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.

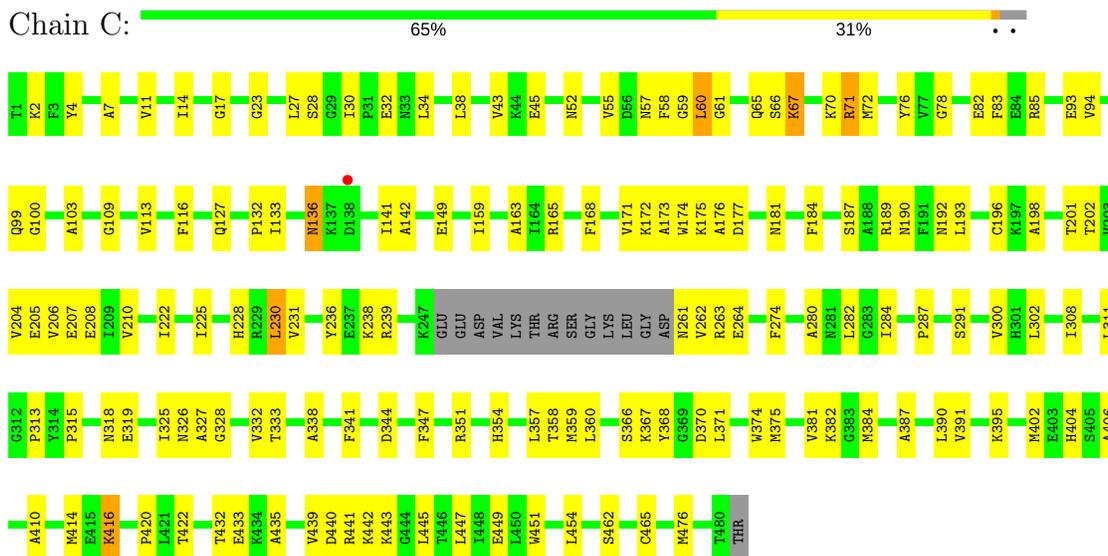
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1



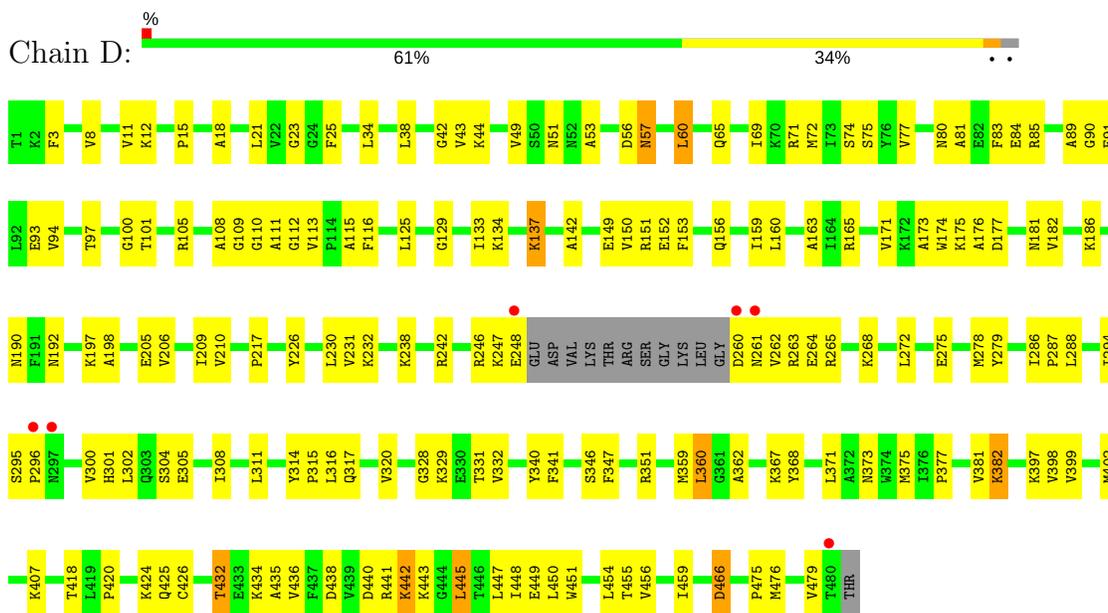
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- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1



- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.97Å 264.43Å 61.42Å 90.00° 109.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.62 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.00) 88.5 (19.62-1.92)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.92Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.275 0.217 , 0.272	Depositor DCC
$R_{free}$ test set	6265 reflections (5.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtrriage
Anisotropy	0.439	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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:  
CL

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	0.59	0/3619	0.82	1/4884 (0.0%)
1	B	0.66	0/3640	0.87	3/4912 (0.1%)
1	C	0.66	0/3619	0.85	2/4884 (0.0%)
1	D	0.61	0/3636	0.83	1/4907 (0.0%)
All	All	0.63	0/14514	0.84	7/19587 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	332	VAL	CB-CA-C	-5.85	100.29	111.40
1	A	216	ALA	N-CA-C	-5.58	95.93	111.00
1	B	73	ILE	N-CA-C	-5.45	96.29	111.00
1	D	316	LEU	N-CA-C	-5.41	96.38	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	3561	0	3636	112	0
1	B	3582	0	3649	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3561	0	3636	120	0
1	D	3578	0	3646	158	0
2	A	1	0	0	0	0
3	A	169	0	0	3	0
3	B	217	0	0	7	0
3	C	242	0	0	8	0
3	D	193	0	0	6	0
All	All	15104	0	14567	491	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 17.

The worst 5 of 491 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:C:384:MET:SD	1:C:384:MET:CE	2.03	1.45
1:B:132:PRO:HB3	1:B:141:ILE:HG12	1.51	0.92
1:A:357:LEU:HD13	1:A:397:LYS:HE3	1.53	0.89
1:D:381:VAL:C	1:D:382:LYS:HE3	1.94	0.88
1:D:42:GLY:O	1:D:44:LYS:HE3	1.75	0.86

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	463/481 (96%)	446 (96%)	15 (3%)	2 (0%)	38 33
1	B	466/481 (97%)	452 (97%)	12 (3%)	2 (0%)	38 33
1	C	463/481 (96%)	450 (97%)	12 (3%)	1 (0%)	51 48
1	D	465/481 (97%)	450 (97%)	14 (3%)	1 (0%)	51 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1857/1924 (96%)	1798 (97%)	53 (3%)	6 (0%)	44 40

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	LYS
1	B	138	ASP
1	B	190	ASN
1	C	190	ASN
1	D	190	ASN

### 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	381/393 (97%)	367 (96%)	14 (4%)	39 36
1	B	383/393 (98%)	369 (96%)	14 (4%)	39 36
1	C	381/393 (97%)	374 (98%)	7 (2%)	64 68
1	D	383/393 (98%)	371 (97%)	12 (3%)	45 44
All	All	1528/1572 (97%)	1481 (97%)	47 (3%)	45 44

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	SER
1	B	414	MET
1	D	432	THR
1	B	341	PHE
1	B	466	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	156	GLN
1	C	301	HIS
1	D	292	ASN
1	C	99	GLN
1	D	99	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 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	467/481 (97%)	-0.15	6 (1%) 77 77	15, 27, 42, 56	0
1	B	470/481 (97%)	-0.31	3 (0%) 89 88	13, 23, 36, 51	0
1	C	467/481 (97%)	-0.34	1 (0%) 94 94	13, 23, 36, 47	0
1	D	469/481 (97%)	-0.10	6 (1%) 77 77	14, 27, 41, 60	0
All	All	1873/1924 (97%)	-0.23	16 (0%) 84 83	13, 25, 40, 60	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	ASP	3.6
1	D	248	GLU	3.4
1	A	480	THR	3.0
1	A	407	LYS	2.9
1	B	297	ASN	2.7

### 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
2	CL	A	901	1/1	0.99	0.03	-3.85	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.