



# wwPDB X-ray Structure Validation Summary Report

Sep 6, 2023 – 07:31 PM EDT

PDB ID : 4GUG  
Title : 1.62 Angstrom Crystal Structure of the Salmonella enterica 3-Dehydroquinase Dehydratase (aroD) E86A Mutant in Complex with Dehydroshikimate (Crystal Form #1)  
Authors : Light, S.H.; Minasov, G.; Duban, M.-E.; Shuvalova, L.; Kwon, K.; Lavie, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-08-29  
Resolution : 1.62 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.35  
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)

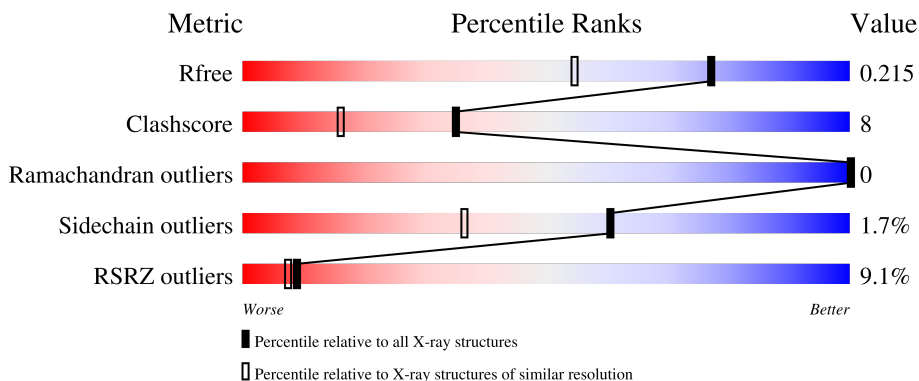
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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))
$R_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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 of 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	276	 2% 74% 14% 11%
1	B	276	 14% 78% 11% 11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4308 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	2030	1289	348	381	12	0	21	0
1	B	245	1890	1197	322	363	8	0	4	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P58687
A	-22	HIS	-	expression tag	UNP P58687
A	-21	HIS	-	expression tag	UNP P58687
A	-20	HIS	-	expression tag	UNP P58687
A	-19	HIS	-	expression tag	UNP P58687
A	-18	HIS	-	expression tag	UNP P58687
A	-17	HIS	-	expression tag	UNP P58687
A	-16	SER	-	expression tag	UNP P58687
A	-15	SER	-	expression tag	UNP P58687
A	-14	GLY	-	expression tag	UNP P58687
A	-13	VAL	-	expression tag	UNP P58687
A	-12	ASP	-	expression tag	UNP P58687
A	-11	LEU	-	expression tag	UNP P58687
A	-10	GLY	-	expression tag	UNP P58687
A	-9	THR	-	expression tag	UNP P58687
A	-8	GLU	-	expression tag	UNP P58687
A	-7	ASN	-	expression tag	UNP P58687
A	-6	LEU	-	expression tag	UNP P58687
A	-5	TYR	-	expression tag	UNP P58687
A	-4	PHE	-	expression tag	UNP P58687
A	-3	GLN	-	expression tag	UNP P58687
A	-2	SER	-	expression tag	UNP P58687
A	-1	ASN	-	expression tag	UNP P58687
A	0	ALA	-	expression tag	UNP P58687
A	86	ALA	GLU	engineered mutation	UNP P58687

*Continued on next page...*

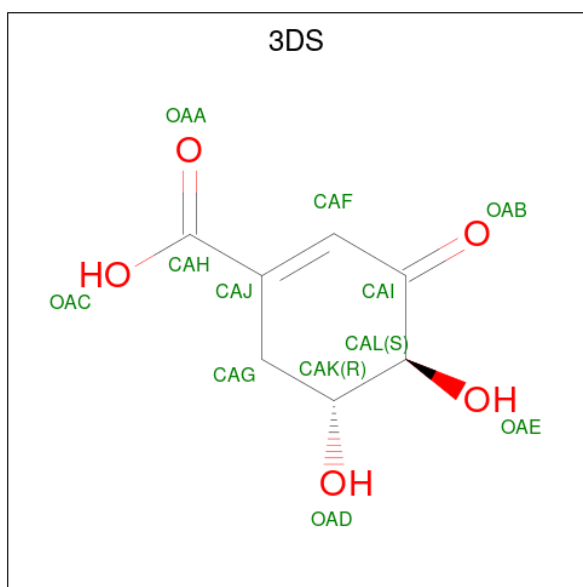
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P58687
B	-22	HIS	-	expression tag	UNP P58687
B	-21	HIS	-	expression tag	UNP P58687
B	-20	HIS	-	expression tag	UNP P58687
B	-19	HIS	-	expression tag	UNP P58687
B	-18	HIS	-	expression tag	UNP P58687
B	-17	HIS	-	expression tag	UNP P58687
B	-16	SER	-	expression tag	UNP P58687
B	-15	SER	-	expression tag	UNP P58687
B	-14	GLY	-	expression tag	UNP P58687
B	-13	VAL	-	expression tag	UNP P58687
B	-12	ASP	-	expression tag	UNP P58687
B	-11	LEU	-	expression tag	UNP P58687
B	-10	GLY	-	expression tag	UNP P58687
B	-9	THR	-	expression tag	UNP P58687
B	-8	GLU	-	expression tag	UNP P58687
B	-7	ASN	-	expression tag	UNP P58687
B	-6	LEU	-	expression tag	UNP P58687
B	-5	TYR	-	expression tag	UNP P58687
B	-4	PHE	-	expression tag	UNP P58687
B	-3	GLN	-	expression tag	UNP P58687
B	-2	SER	-	expression tag	UNP P58687
B	-1	ASN	-	expression tag	UNP P58687
B	0	ALA	-	expression tag	UNP P58687
B	86	ALA	GLU	engineered mutation	UNP P58687

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

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

- Molecule 3 is (4S,5R)-4,5-dihydroxy-3-oxocyclohex-1-ene-1-carboxylic acid (three-letter code: 3DS) (formula: C<sub>7</sub>H<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 7 5	0	1
3	B	1	Total C O 11 7 4	0	0

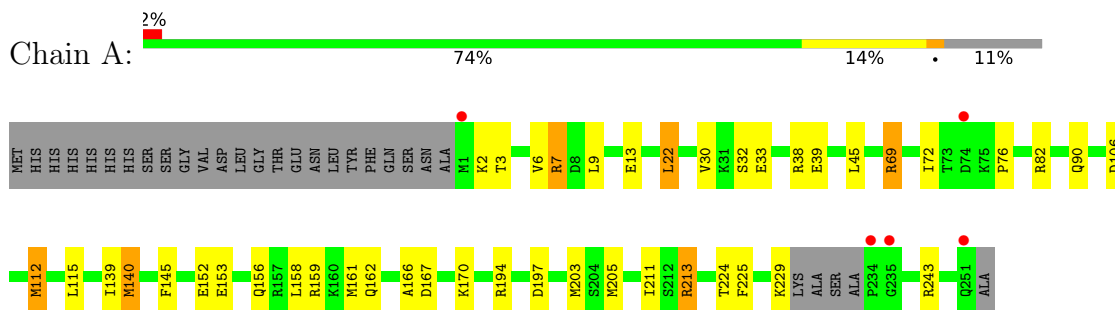
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	247	Total O 252 252	0	5
4	B	112	Total O 112 112	0	0

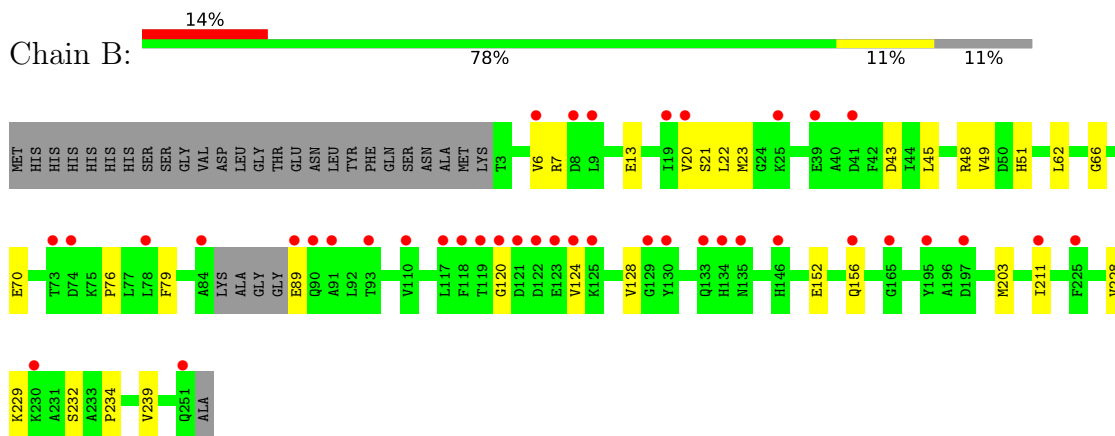
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.70Å 64.27Å 81.05Å 90.00° 93.89° 90.00°	Depositor
Resolution (Å)	29.86 – 1.62 29.86 – 1.62	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.86-1.62) 97.1 (29.86-1.62)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 1.62Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.173 , 0.208 0.183 , 0.215	Depositor DCC
$R_{free}$ test set	2908 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.3	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	0.97	EDS
Total number of atoms	4308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, 3DS

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	1.12	4/2091 (0.2%)	1.14	11/2823 (0.4%)
1	B	0.79	0/1928	0.89	1/2615 (0.0%)
All	All	0.97	4/4019 (0.1%)	1.03	12/5438 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLU	CD-OE2	6.03	1.32	1.25
1	A	32	SER	CB-OG	-5.74	1.34	1.42
1	A	243	ARG	CZ-NH2	-5.06	1.26	1.33
1	A	213	ARG	CZ-NH1	5.01	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140[A]	MET	CG-SD-CE	-9.62	84.81	100.20
1	A	140[B]	MET	CG-SD-CE	-9.62	84.81	100.20
1	A	69[A]	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	69[B]	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	106	ASP	CB-CG-OD2	6.06	123.76	118.30

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	2030	0	2124	46	4
1	B	1890	0	1936	23	0
2	A	1	0	0	0	0
3	A	12	0	7	0	0
3	B	11	0	7	0	0
4	A	252	0	0	12	0
4	B	112	0	0	4	0
All	All	4308	0	4074	66	4

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 8.

The worst 5 of 66 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:2[A]:LYS:CD	4:A:547:HOH:O	2.01	1.07
1:A:2[A]:LYS:HD3	4:A:547:HOH:O	1.59	1.02
1:A:211:ILE:HD11	1:B:211:ILE:HD11	1.48	0.96
1:B:20[B]:VAL:HG21	1:B:228:VAL:HG23	1.55	0.89
1:A:2[A]:LYS:HD2	4:A:547:HOH:O	1.69	0.88

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE2	1:A:194[B]:ARG:NH1[1_655]	1.16	1.04
1:A:39:GLU:OE1	1:A:194[B]:ARG:NH2[1_655]	1.51	0.69
1:A:39:GLU:OE2	1:A:194[B]:ARG:CZ[1_655]	1.75	0.45
1:A:39:GLU:CD	1:A:194[B]:ARG:NH1[1_655]	1.85	0.35

## 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	264/276 (96%)	258 (98%)	6 (2%)	0	100	100
1	B	245/276 (89%)	237 (97%)	8 (3%)	0	100	100
All	All	509/552 (92%)	495 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	223/225 (99%)	220 (99%)	3 (1%)	69	49
1	B	205/225 (91%)	200 (98%)	5 (2%)	49	22
All	All	428/450 (95%)	420 (98%)	8 (2%)	60	32

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	234	PRO
1	B	229	LYS
1	B	89	GLU
1	B	13	GLU
1	B	203	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	B	143	HIS
1	B	251	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
3	3DS	B	301	1	11,11,12	1.37	2 (18%)	12,15,17	2.19	5 (41%)
3	3DS	A	302[A]	-	12,12,12	2.36	5 (41%)	14,17,17	1.60	3 (21%)

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	3DS	B	301	1	-	4/4/17/20	0/1/1/1
3	3DS	A	302[A]	-	-	4/4/20/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	3DS	CAK-CAL	4.55	1.57	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	3DS	OAB-CAI	4.22	1.28	1.22
3	B	301	3DS	CAI-CAL	-3.07	1.48	1.52
3	A	302[A]	3DS	CAL-CAI	-2.79	1.50	1.52
3	A	302[A]	3DS	CAH-CAJ	-2.37	1.43	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	3DS	OAA-CAH-CAJ	-5.17	112.68	121.59
3	B	301	3DS	OAD-CAK-CAL	-2.93	103.73	110.22
3	A	302[A]	3DS	CAG-CAK-CAL	2.91	112.86	109.24
3	A	302[A]	3DS	OAE-CAL-CAI	2.83	116.17	111.31
3	A	302[A]	3DS	OAD-CAK-CAL	2.61	114.13	109.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	3DS	OAA-CAH-CAJ-CAF
3	A	302[A]	3DS	OAC-CAH-CAJ-CAF
3	B	301	3DS	OAA-CAH-CAJ-CAF
3	B	301	3DS	OAA-CAH-CAJ-CAG
3	B	301	3DS	OAC-CAH-CAJ-CAF

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	247/276 (89%)	0.02	5 (2%) 65 63	16, 25, 45, 70	0
1	B	245/276 (88%)	0.74	40 (16%) 1 1	25, 42, 71, 102	0
All	All	492/552 (89%)	0.38	45 (9%) 9 7	16, 33, 68, 102	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	GLN	5.9
1	B	122	ASP	5.8
1	B	118	PHE	5.2
1	B	130	TYR	5.2
1	A	234	PRO	4.8

### 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 monosaccharides 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. 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( $\text{\AA}^2$ )	Q<0.9
3	3DS	A	302[A]	12/12	0.88	0.24	23,25,32,33	12
3	3DS	B	301	11/12	0.88	0.33	26,29,32,33	11
2	CL	A	301	1/1	0.98	0.04	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.