



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:06 PM GMT

PDB ID : 3W1H  
Title : Crystal structure of the selenocysteine synthase SelA from Aquifex aeolicus  
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.  
Deposited on : 2012-11-15  
Resolution : 3.89 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

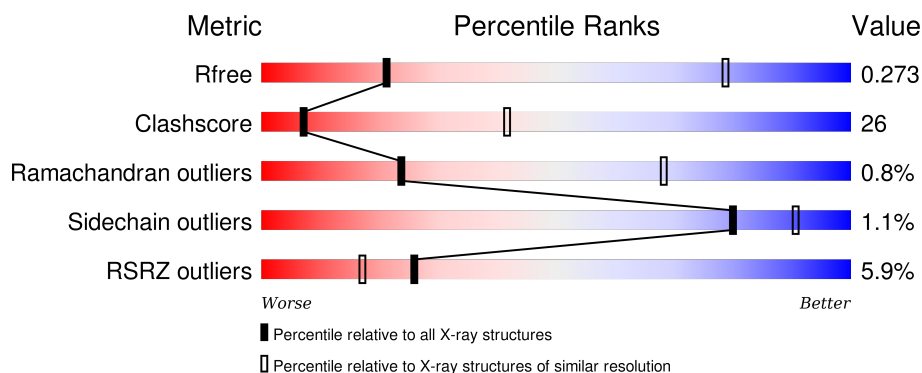
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.89 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	452	<div> <div>6%</div> <div> <div></div> <div>53%</div> <div>46%</div> <div></div> </div> <div></div> </div>
1	B	452	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div></div> </div> <div></div> </div>
1	C	452	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>49%</div> <div></div> </div> <div></div> </div>
1	D	452	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>42%</div> <div></div> </div> <div>13%</div> </div>
1	E	452	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>37%</div> <div></div> </div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	LLP	B	285	-	-	X	-

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16913 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	443	Total	C	N	O	P	S	0	0	0
			3501	2230	606	654	1	10			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	395	Total	C	N	O	P	S	0	0	0
			3115	1980	542	582	1	10			
1	E	399	Total	C	N	O	P	S	0	0	0
			3147	2000	546	590	1	10			

There are 20 discrepancies between the modelled and reference sequences:

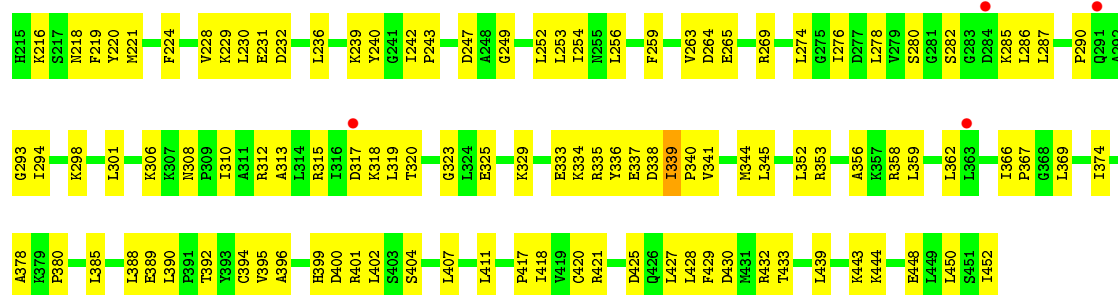
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140

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Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140

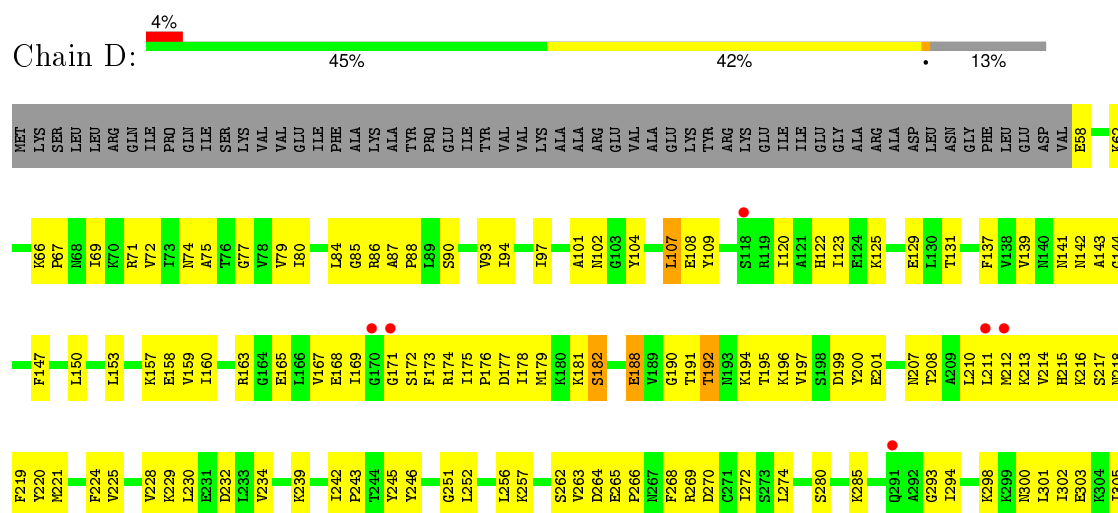


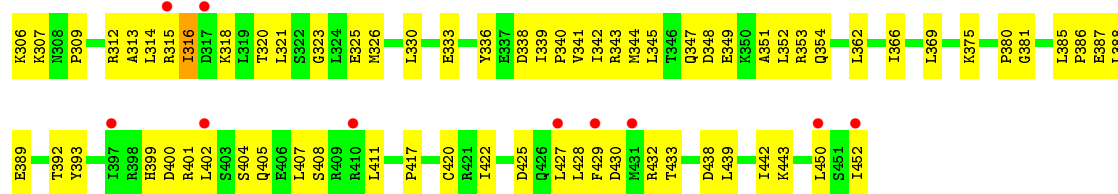


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

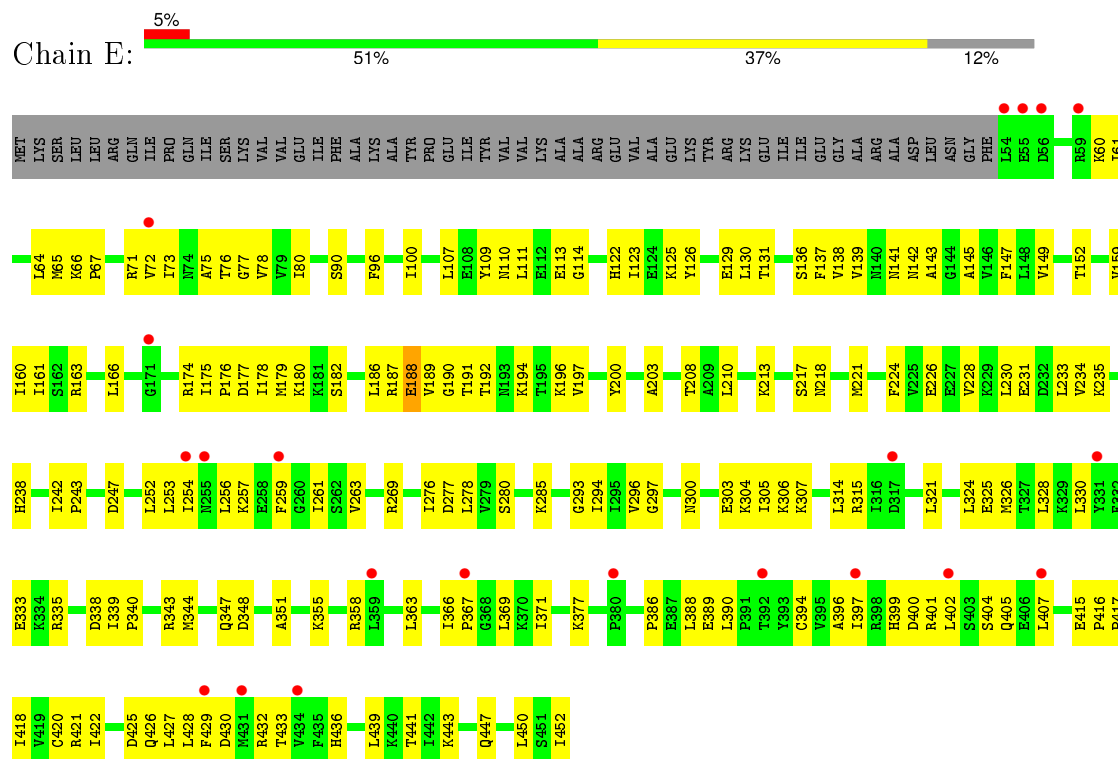


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase





• Molecule 1: L-seryl-tRNA(Sec) selenium transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.03Å 167.03Å 211.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.89 49.25 – 3.89	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.25-3.89) 94.2 (49.25-3.89)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.220 , 0.282 0.202 , 0.273	Depositor DCC
$R_{free}$ test set	1344 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	130.3	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 135.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 26371 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: LLP

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	0/3597	0.62	0/4831
1	B	0.43	0/3522	0.64	0/4731
1	C	0.41	0/3597	0.62	0/4831
1	D	0.38	0/3130	0.60	0/4203
1	E	0.41	0/3162	0.60	0/4247
All	All	0.41	0/17008	0.62	0/22843

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	3575	0	3761	215	0
1	B	3501	0	3670	235	0
1	C	3575	0	3761	223	0
1	D	3115	0	3273	185	0
1	E	3147	0	3303	145	0
All	All	16913	0	17768	910	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 910 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:102:ASN:HB3	1:D:71:ARG:HH22	1.16	1.03
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.41	1.03
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.37	1.02
1:A:69:ILE:HG22	1:B:100:ILE:HD12	1.49	0.95
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.31	0.94

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	449/452 (99%)	417 (93%)	29 (6%)	3 (1%)	26	70
1	B	440/452 (97%)	403 (92%)	31 (7%)	6 (1%)	14	58
1	C	449/452 (99%)	409 (91%)	36 (8%)	4 (1%)	21	65
1	D	392/452 (87%)	366 (93%)	22 (6%)	4 (1%)	19	64
1	E	396/452 (88%)	374 (94%)	22 (6%)	0	100	100
All	All	2126/2260 (94%)	1969 (93%)	140 (7%)	17 (1%)	24	68

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	B	107	LEU
1	C	192	THR
1	A	107	LEU
1	A	192	THR

### 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	390/390 (100%)	384 (98%)	6 (2%)	72	89
1	B	381/390 (98%)	375 (98%)	6 (2%)	70	88
1	C	390/390 (100%)	387 (99%)	3 (1%)	86	93
1	D	342/390 (88%)	338 (99%)	4 (1%)	78	90
1	E	346/390 (89%)	344 (99%)	2 (1%)	90	95
All	All	1849/1950 (95%)	1828 (99%)	21 (1%)	80	90

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	SER
1	B	339	ILE
1	D	188	GLU
1	B	169	ILE
1	D	316	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	405	GLN
1	D	238	HIS
1	E	405	GLN
1	C	436	HIS
1	D	122	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	LLP	A	285	1	23,24,25	1.67	6 (26%)	28,32,34	1.61	3 (10%)
1	LLP	B	285	1	23,24,25	1.53	4 (17%)	28,32,34	1.48	4 (14%)
1	LLP	C	285	1	23,24,25	1.58	4 (17%)	28,32,34	1.69	3 (10%)
1	LLP	D	285	1	23,24,25	1.66	7 (30%)	28,32,34	1.61	2 (7%)
1	LLP	E	285	1	23,24,25	1.74	4 (17%)	28,32,34	1.60	5 (17%)

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
1	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1
1	LLP	E	285	1	-	0/15/17/19	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	285	LLP	CE-NZ	-3.40	1.39	1.46
1	A	285	LLP	C3-C2	-3.21	1.38	1.40
1	A	285	LLP	CE-NZ	-2.51	1.41	1.46
1	B	285	LLP	C3-C2	-2.48	1.39	1.40
1	D	285	LLP	CE-NZ	-2.32	1.42	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LLP	O-C-CA	-3.14	117.31	125.49
1	B	285	LLP	C5-C6-N1	-2.75	119.08	123.86
1	E	285	LLP	C3-C4-C4'	-2.72	116.64	120.16
1	D	285	LLP	O-C-CA	-2.53	118.90	125.49
1	E	285	LLP	O-C-CA	-2.34	119.38	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	3	0
1	B	285	LLP	9	0
1	C	285	LLP	5	0
1	D	285	LLP	3	0
1	E	285	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	451/452 (99%)	0.34	26 (5%) 26 18	127, 198, 298, 335	0
1	B	442/452 (97%)	0.26	31 (7%) 19 13	120, 186, 310, 350	0
1	C	451/452 (99%)	0.31	31 (6%) 20 13	122, 198, 299, 337	0
1	D	394/452 (87%)	0.21	16 (4%) 41 30	134, 192, 274, 309	0
1	E	398/452 (88%)	0.14	21 (5%) 30 22	156, 222, 312, 372	0
All	All	2136/2260 (94%)	0.26	125 (5%) 26 17	120, 199, 301, 372	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.1
1	C	451	SER	6.4
1	C	9	PRO	6.0
1	B	17	ILE	5.3
1	C	1	MET	5.2

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

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
1	LLP	E	285	24/25	0.86	0.36	-	176,200,215,225	0
1	LLP	B	285	24/25	0.92	0.34	-	123,153,174,176	0
1	LLP	C	285	24/25	0.92	0.33	-	113,163,182,192	0
1	LLP	A	285	24/25	0.92	0.38	-	136,182,191,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	D	285	24/25	0.93	0.30	-	146,165,183,193	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.