



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:30 AM GMT

PDB ID : 2HFB  
Title : Crystal structure of selenomethionine-labelled RafE from *Streptococcus pneumoniae*  
Authors : Paterson, N.G.; Riboldi-Tunncliffe, A.; Mitchell, T.J.; Isaacs, N.W.  
Deposited on : 2006-06-23  
Resolution : 2.90 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

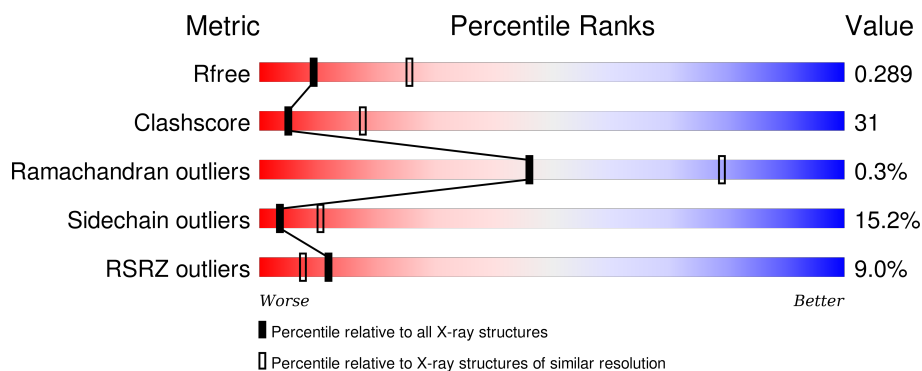
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	409	<div> <div>15%</div> <div>48%</div> <div>38%</div> <div>7%</div> <div>6%</div> </div>
1	B	409	<div> <div>15%</div> <div>46%</div> <div>37%</div> <div>10%</div> <div>7%</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
2	CL	A	401	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6045 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 Sugar ABC transporter, sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	Se	69	0	0
			3029	1937	497	584	11			
1	B	381	Total	C	N	O	Se	376	0	0
			3013	1927	494	581	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	CLONING ARTIFACT	UNP Q97NW2
A	-16	ARG	-	CLONING ARTIFACT	UNP Q97NW2
A	-15	GLY	-	CLONING ARTIFACT	UNP Q97NW2
A	-14	SER	-	CLONING ARTIFACT	UNP Q97NW2
A	-13	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-12	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-11	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-10	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-9	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-8	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-7	THR	-	CLONING ARTIFACT	UNP Q97NW2
A	-6	ASP	-	CLONING ARTIFACT	UNP Q97NW2
A	-5	PRO	-	CLONING ARTIFACT	UNP Q97NW2
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	201	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	208	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	240	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	264	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	302	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	308	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	336	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	364	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	375	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	386	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	-17	MET	-	CLONING ARTIFACT	UNP Q97NW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	ARG	-	CLONING ARTIFACT	UNP Q97NW2
B	-15	GLY	-	CLONING ARTIFACT	UNP Q97NW2
B	-14	SER	-	CLONING ARTIFACT	UNP Q97NW2
B	-13	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-12	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-11	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-10	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-9	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-8	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-7	THR	-	CLONING ARTIFACT	UNP Q97NW2
B	-6	ASP	-	CLONING ARTIFACT	UNP Q97NW2
B	-5	PRO	-	CLONING ARTIFACT	UNP Q97NW2
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	201	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	208	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	240	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	264	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	302	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	308	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	336	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	364	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	375	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	386	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2

- 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

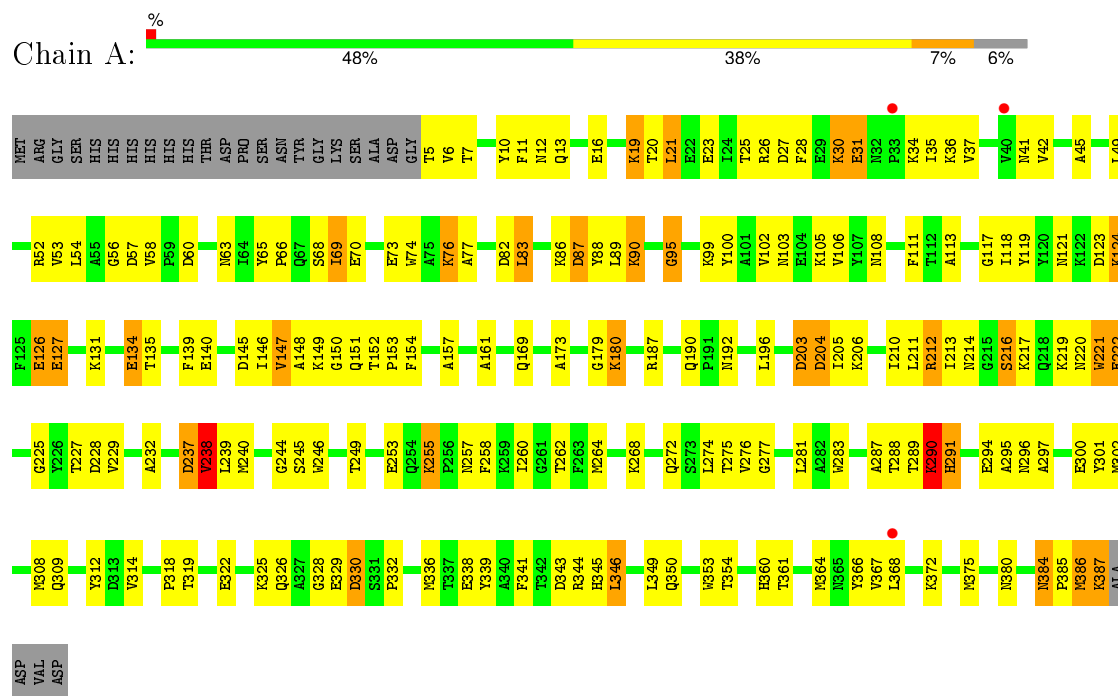
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0

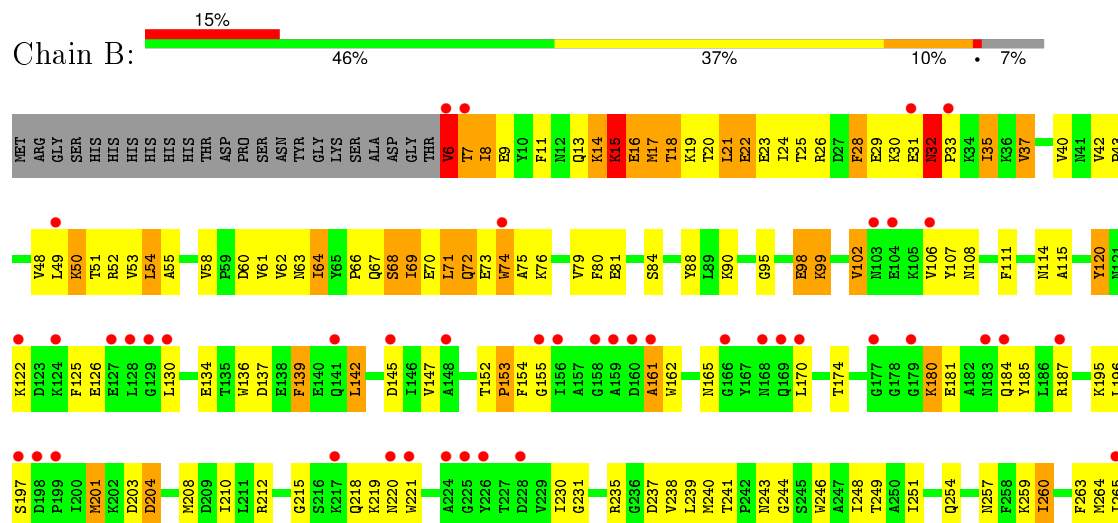
### 3 Residue-property plots

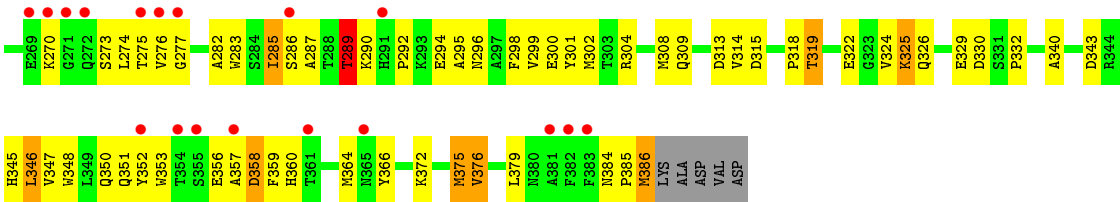
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Sugar ABC transporter, sugar-binding protein



- Molecule 1: Sugar ABC transporter, sugar-binding protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.54Å 144.54Å 224.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.51 – 2.90 29.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.51-2.90) 99.2 (29.51-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.50 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.248 , 0.290 0.244 , 0.289	Depositor DCC
$R_{free}$ test set	1568 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 31023 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: 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	1.20	7/3088 (0.2%)	1.15	18/4168 (0.4%)
1	B	0.95	11/3072 (0.4%)	1.24	25/4147 (0.6%)
All	All	1.08	18/6160 (0.3%)	1.20	43/8315 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	4
All	All	1	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE2	8.71	1.35	1.25
1	B	185	TYR	CB-CG	-7.77	1.40	1.51
1	B	16	GLU	CG-CD	7.26	1.62	1.51
1	A	322	GLU	CB-CG	7.05	1.65	1.52
1	A	36	LYS	CA-CB	-6.96	1.38	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	TYR	CB-CG-CD1	-27.10	104.74	121.00
1	B	185	TYR	CB-CG-CD2	26.29	136.78	121.00
1	B	28	PHE	CB-CA-C	-9.38	91.63	110.40
1	A	344	ARG	NE-CZ-NH2	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ALA	CB-CA-C	-8.30	97.64	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	386	MSE	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	GLY	Peptide
1	B	154	PHE	Peptide
1	B	289	THR	Peptide
1	B	32	ASN	Peptide
1	B	6	VAL	Peptide

## 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	3029	0	2968	165	0
1	B	3013	0	2948	182	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
All	All	6045	0	5916	338	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 31.

The worst 5 of 338 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:B:187:ARG:O	1:B:187:ARG:HD2	1.43	1.15
1:A:387:LYS:O	1:A:387:LYS:HE2	1.44	1.14
1:A:6:VAL:HG11	1:A:291:HIS:CD2	1.81	1.14
1:B:62:VAL:HG23	1:B:64:ILE:HG22	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:O	1:B:35:ILE:HG13	1.48	1.11

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	381/409 (93%)	339 (89%)	41 (11%)	1 (0%)	46	79
1	B	379/409 (93%)	325 (86%)	53 (14%)	1 (0%)	46	79
All	All	760/818 (93%)	664 (87%)	94 (12%)	2 (0%)	46	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	B	55	ALA

### 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	320/330 (97%)	280 (88%)	40 (12%)	6	17
1	B	318/330 (96%)	261 (82%)	57 (18%)	2	6
All	All	638/660 (97%)	541 (85%)	97 (15%)	3	10

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	LYS
1	B	50	LYS
1	B	330	ASP
1	B	17	MSE
1	B	25	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	384	ASN
1	B	309	GLN
1	A	309	GLN
1	B	326	GLN

### 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 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	372/409 (90%)	-0.21	3 (0%) 87 86	20, 67, 112, 160	19 (5%)
1	B	350/409 (85%)	0.75	62 (17%) 2 1	68, 121, 206, 241	51 (14%)
All	All	722/818 (88%)	0.26	65 (9%) 12 7	20, 88, 194, 241	70 (9%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	ALA	5.7
1	B	383	PHE	5.5
1	B	381	ALA	5.1
1	B	265	ILE	4.9
1	B	382	PHE	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( $\text{\AA}^2$ )	Q<0.9
2	CL	A	401	1/1	0.97	0.24	5.88	63,63,63,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.