

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 16, 2023 – 02:53 AM EDT

PDB ID 1YLK

> Title Crystal Structure of Rv1284 from Mycobacterium tuberculosis in Complex

> > with Thiocyanate

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Europe (SPINE)

Deposited on 2005-01-19

Resolution 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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 (i) 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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

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)

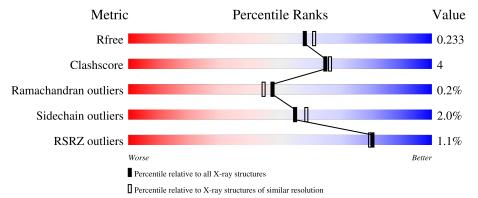
Validation Pipeline (wwPDB-VP) 2.35

## 1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	172	90%	5% 5%
1	В	172	85%	9% • 5%
1	С	172	83%	10% • 5%
1	D	172	83%	12% • 5%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5371 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 Hypothetical protein Rv1284/MT1322.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	163	Total	С	N	О	S	0	0	0
1	A	105	1271	798	224	242	7	0	U	U
1	В	163	Total	С	N	О	S	0	0	0
1	Б	105	1271	798	224	242	7	U		
1	C	163	Total	С	N	О	S	0	0	0
1		105	1271	798	224	242	7	0	U	U
1	1 D	162	Total	С	N	О	S	0	0	0
	163	1271	798	224	242	7		0	U	

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	cloning artifact	UNP P64797
A	-7	ALA	-	cloning artifact	UNP P64797
A	-6	HIS	-	cloning artifact	UNP P64797
A	-5	HIS	-	cloning artifact	UNP P64797
A	-4	HIS	-	cloning artifact	UNP P64797
A	-3	HIS	-	cloning artifact	UNP P64797
A	-2	HIS	-	cloning artifact	UNP P64797
A	-1	HIS	-	cloning artifact	UNP P64797
A	0	SER	ı	cloning artifact	UNP P64797
A	1	GLY	-	cloning artifact	UNP P64797
В	-8	MET	ı	cloning artifact	UNP P64797
В	-7	ALA	ı	cloning artifact	UNP P64797
В	-6	HIS	-	cloning artifact	UNP P64797
В	-5	HIS	ı	cloning artifact	UNP P64797
В	-4	HIS	-	cloning artifact	UNP P64797
В	-3	HIS	-	cloning artifact	UNP P64797
В	-2	HIS	-	cloning artifact	UNP P64797
В	-1	HIS		cloning artifact	UNP P64797
В	0	SER	=	cloning artifact	UNP P64797
В	1	GLY		cloning artifact	UNP P64797
С	-8	MET	-	cloning artifact	UNP P64797

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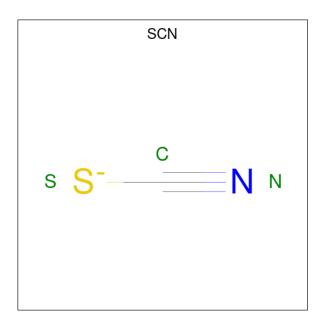
Chain	Residue	Modelled	Actual	Comment	Reference
С	-7	ALA	-	cloning artifact	UNP P64797
С	-6	HIS	-	cloning artifact	UNP P64797
С	-5	HIS	-	cloning artifact	UNP P64797
С	-4	HIS	-	cloning artifact	UNP P64797
С	-3	HIS	-	cloning artifact	UNP P64797
С	-2	HIS	-	cloning artifact	UNP P64797
С	-1	HIS	-	cloning artifact	UNP P64797
С	0	SER	-	cloning artifact	UNP P64797
С	1	GLY	-	cloning artifact	UNP P64797
D	-8	MET	-	cloning artifact	UNP P64797
D	-7	ALA	-	cloning artifact	UNP P64797
D	-6	HIS	-	cloning artifact	UNP P64797
D	-5	HIS	-	cloning artifact	UNP P64797
D	-4	HIS	-	cloning artifact	UNP P64797
D	-3	HIS	-	cloning artifact	UNP P64797
D	-2	HIS	-	cloning artifact	UNP P64797
D	-1	HIS	-	cloning artifact	UNP P64797
D	0	SER	-	cloning artifact	UNP P64797
D	1	GLY	-	cloning artifact	UNP P64797

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

• Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Δ	1	Total C N S	0	0	
	11	1	3 1 1 1	U	U	
3	A	1	Total C N S	0	0	
	11	1	3 1 1 1	U	U	
3	В	1	Total C N S	0	0	
J	D	1	3 1 1 1	U		
3	С	1	Total C N S	0	0	
J		1	3 1 1 1	U	U	
3	C	1	Total C N S	0	0	
9		1	3 1 1 1		U	

#### • Molecule 4 is water.

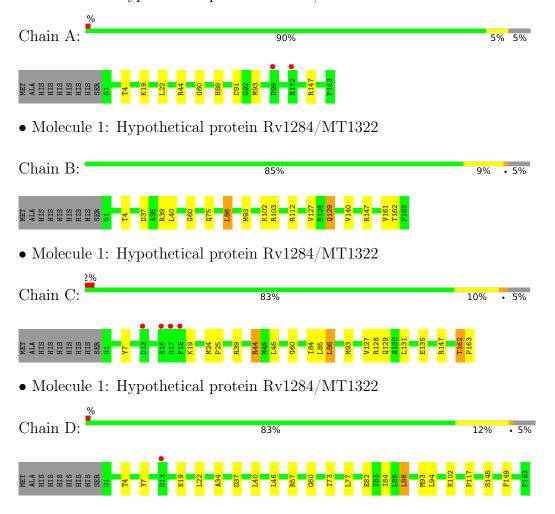
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	В	68	Total O 68 68	0	0
4	С	65	Total O 65 65	0	0
4	D	73	Total O 73 73	0	0



## 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: Hypothetical protein Rv1284/MT1322





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants	100.16Å 154.07Å 156.94Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	42.26 - 2.00	Depositor
Resolution (A)	42.22 - 2.00	EDS
% Data completeness	94.2 (42.26-2.00)	Depositor
(in resolution range)	94.2 (42.22-2.00)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	6.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.181 , 0.226	Depositor
$R, R_{free}$	0.194 , $0.233$	DCC
$R_{free}$ test set	1946 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.42 , 51.5	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 22.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8089e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: SCN, ZN

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).

Mal	Clasia	Bond	lengths	Bond angles		
Mol	Chain	RMSZ   # Z  > 5		RMSZ	# Z  > 5	
1	A	0.51	0/1296	0.63	0/1761	
1	В	0.50	0/1296	0.66	1/1761 (0.1%)	
1	С	0.49	0/1296	0.64	0/1761	
1	D	0.48	0/1296	0.62	1/1761 (0.1%)	
All	All	0.50	0/5184	0.64	2/7044 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	В	86	LEU	CA-CB-CG	5.35	127.60	115.30
1	D	94	LEU	CA-CB-CG	5.30	127.48	115.30

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	1271	0	1263	6	0
1	В	1271	0	1263	13	0
1	С	1271	0	1263	17	0
1	D	1271	0	1263	13	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0
3	В	3	0	0	0	0
3	С	6	0	0	0	0
4	A	62	0	0	1	0
4	В	68	0	0	2	0
4	С	65	0	0	0	0
4	D	73	0	0	1	0
All	All	5371	0	5052	42	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (42) 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:140:VAL:HG12	1:B:140:VAL:O	1.72	0.87
1:C:128:ARG:HE	1:C:163:PRO:CD	1.99	0.76
1:C:128:ARG:HE	1:C:163:PRO:HD2	1.57	0.68
1:B:60:GLY:HA3	1:B:93:MET:HG3	1.75	0.67
1:A:60:GLY:HA3	1:A:93:MET:HG3	1.82	0.61
1:B:140:VAL:O	1:B:140:VAL:CG1	2.45	0.59
1:B:75:GLN:NE2	4:B:564:HOH:O	2.27	0.56
1:C:60:GLY:HA3	1:C:93:MET:HG3	1.87	0.56
1:C:84:ILE:HG22	1:C:86:LEU:HD13	1.86	0.56
1:C:127:VAL:O	1:C:131:LEU:HG	2.07	0.55
1:D:60:GLY:HA3	1:D:93:MET:HG3	1.89	0.55
1:C:7:TYR:HB3	1:D:46:LEU:HD22	1.89	0.53
1:D:37:ASP:HB3	1:D:40:LEU:HD13	1.91	0.52
1:C:128:ARG:NE	1:C:163:PRO:HD2	2.25	0.49
1:B:102:LYS:NZ	4:B:567:HOH:O	2.28	0.48
1:C:84:ILE:CG2	1:C:86:LEU:HD13	2.44	0.48
1:D:73:ILE:HG23	1:D:77:LEU:HD12	1.97	0.47
1:A:44:ARG:NH2	4:A:551:HOH:O	2.48	0.46
1:C:39:ARG:HG2	1:D:22:LEU:HB2	1.98	0.45
1:A:88:HIS:CE1	1:A:91:CYS:HA	2.51	0.45
1:D:84:ILE:HG22	1:D:86:LEU:HD13	1.98	0.45
1:B:60:GLY:HA3	1:B:93:MET:CG	2.46	0.45
1:A:22:LEU:HB2	1:B:39:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:D:34:ALA:O	1:D:57:ARG:HA	2.17	0.44
1:A:4:THR:HG21	1:B:147:ARG:HD3	1.98	0.44
1:C:44:ARG:NE	1:C:44:ARG:HA	2.32	0.44
1:B:127:VAL:HG11	1:B:161:VAL:HB	2.00	0.43
1:C:46:LEU:HD22	1:D:7:TYR:HB3	2.01	0.42
1:D:82:GLU:HG2	1:D:145:SER:HB3	2.01	0.42
1:C:24:MET:HB3	1:C:25:PRO:HD3	2.00	0.41
1:C:131:LEU:O	1:C:135:GLU:HG3	2.19	0.41
1:B:102:LYS:HD3	1:B:112:ARG:HG3	2.01	0.41
1:D:102:LYS:HE3	1:D:117:PRO:HD3	2.02	0.41
1:C:85:LEU:HD12	1:C:131:LEU:HD23	2.03	0.41
1:D:86:LEU:HD12	1:D:149:PHE:HB2	2.03	0.41
1:D:102:LYS:NZ	4:D:475:HOH:O	2.26	0.41
1:C:147:ARG:HD3	1:D:4:THR:HG21	2.04	0.40
1:C:162:THR:HB	1:C:163:PRO:HD3	2.02	0.40
1:B:129:GLN:HE21	1:B:129:GLN:HB3	1.77	0.40
1:B:37:ASP:HB3	1:B:40:LEU:HD13	2.02	0.40
1:A:147:ARG:HD3	1:B:4:THR:HG21	2.02	0.40
1:C:128:ARG:HE	1:C:163:PRO:CG	2.35	0.40

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	Perce	ntiles
1	A	161/172 (94%)	157 (98%)	4 (2%)	0	100	100
1	В	161/172 (94%)	159 (99%)	2 (1%)	0	100	100
1	С	161/172 (94%)	157 (98%)	3 (2%)	1 (1%)	25	19
1	D	161/172 (94%)	158 (98%)	3 (2%)	0	100	100
All	All	644/688 (94%)	631 (98%)	12 (2%)	1 (0%)	47	44



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	$\mathbf{C}$	162	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	F	erce	entiles
1	A	141/149~(95%)	140 (99%)	1 (1%)		84	88
1	В	141/149~(95%)	137 (97%)	4 (3%)		43	44
1	С	141/149~(95%)	137 (97%)	4 (3%)		43	44
1	D	141/149~(95%)	139 (99%)	2 (1%)		67	72
All	All	564/596~(95%)	553 (98%)	11 (2%)		55	58

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	В	86	LEU
1	В	103	ARG
1	В	129	GLN
1	В	162	THR
1	С	19	LYS
1	С	44	ARG
1	С	86	LEU
1	С	129	GLN
1	D	19	LYS
1	D	86	LEU

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	143	HIS
1	В	29	HIS
1	В	143	HIS



#### 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	Chain	Res	Link	В	ond len	$\operatorname{gths}$	В	ond ang	gles
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	SCN	С	503	-	1,2,2	2.11	1 (100%)	0,1,1	_	-	
3	SCN	A	505	-	1,2,2	0.89	0	0,1,1	-	-	
3	SCN	A	502	-	1,2,2	1.26	0	0,1,1	-	-	
3	SCN	С	504	-	1,2,2	1.03	0	0,1,1	-	-	
3	SCN	В	501	-	1,2,2	0.76	0	0,1,1	_	-	

#### All (1) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
3	С	503	SCN	C-N	2.11	1.22	1.15

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,  $95^{th}$  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>	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	163/172 (94%)	-0.21	2 (1%) 79 78	17, 22, 29, 35	1 (0%)
1	В	163/172 (94%)	-0.22	0 100 100	17, 22, 29, 32	0
1	С	163/172 (94%)	-0.19	4 (2%) 57 56	18, 22, 30, 35	0
1	D	163/172 (94%)	-0.23	1 (0%) 89 88	17, 22, 29, 32	0
All	All	$652/688 \; (94\%)$	-0.21	7 (1%) 80 79	17, 22, 29, 35	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	17	GLY	2.5
1	С	16	SER	2.5
1	С	13	ASP	2.3
1	A	132	ARG	2.2
1	С	18	PHE	2.2
1	D	13	ASP	2.1
1	A	99	ASP	2.1

### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	SCN	С	504	3/3	0.92	0.09	36,36,37,37	0
3	SCN	С	503	3/3	0.93	0.12	35,35,35,36	0
3	SCN	A	502	3/3	0.94	0.13	39,39,39,39	0
3	SCN	В	501	3/3	0.94	0.09	34,34,34,34	0
3	SCN	A	505	3/3	0.97	0.08	45,45,45,46	0
2	ZN	В	402	1/1	0.99	0.04	33,33,33,33	0
2	ZN	С	403	1/1	0.99	0.05	31,31,31,31	0
2	ZN	D	404	1/1	0.99	0.03	31,31,31,31	0
2	ZN	A	401	1/1	0.99	0.06	32,32,32,32	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

