



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:05 PM GMT

PDB ID : 1WE5  
Title : Crystal Structure of Alpha-Xylosidase from Escherichia coli  
Authors : Ose, T.; Kitamura, M.; Okuyama, M.; Mori, H.; Kimura, A.; Watanabe, N.; Yao, M.; Tanaka, I.  
Deposited on : 2004-05-24  
Resolution : 2.40 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

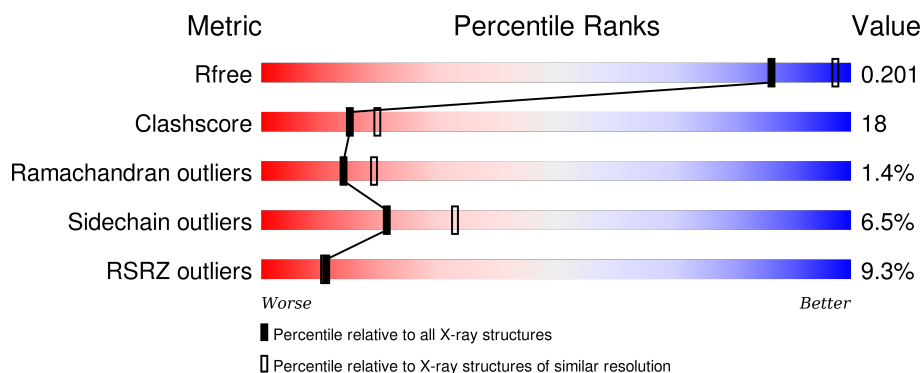
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	772	<div> <div>11%</div> <div>68%28%.</div> </div>
1	B	772	<div> <div>9%</div> <div>65%29%..</div> </div>
1	C	772	<div> <div>6%</div> <div>65%28%5%.</div> </div>
1	D	772	<div> <div>8%</div> <div>66%28%..</div> </div>
1	E	772	<div> <div>10%</div> <div>64%30%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	772	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37302 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	Se	0	0	0
			6222	3975	1068	1147	13	19			
1	B	760	Total	C	N	O	S	Se	0	0	0
			6121	3909	1051	1129	13	19			
1	C	756	Total	C	N	O	S	Se	0	0	0
			6093	3891	1047	1123	13	19			
1	D	757	Total	C	N	O	S	Se	0	0	0
			6096	3892	1047	1125	13	19			
1	E	755	Total	C	N	O	S	Se	0	0	0
			6086	3887	1045	1122	13	19			
1	F	757	Total	C	N	O	S	Se	0	0	0
			6094	3891	1047	1124	13	19			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	593	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
A	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	32	MSE	MET	MODIFIED RESIDUE	UNP P31434

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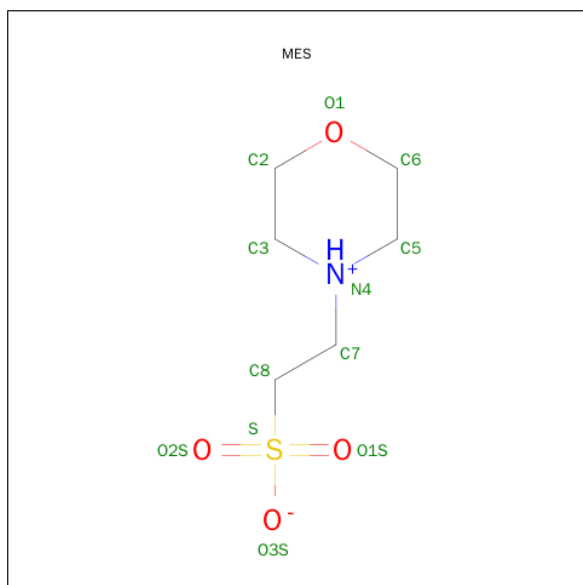
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	310	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
F	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	615	MSE	MET	MODIFIED RESIDUE	UNP P31434

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

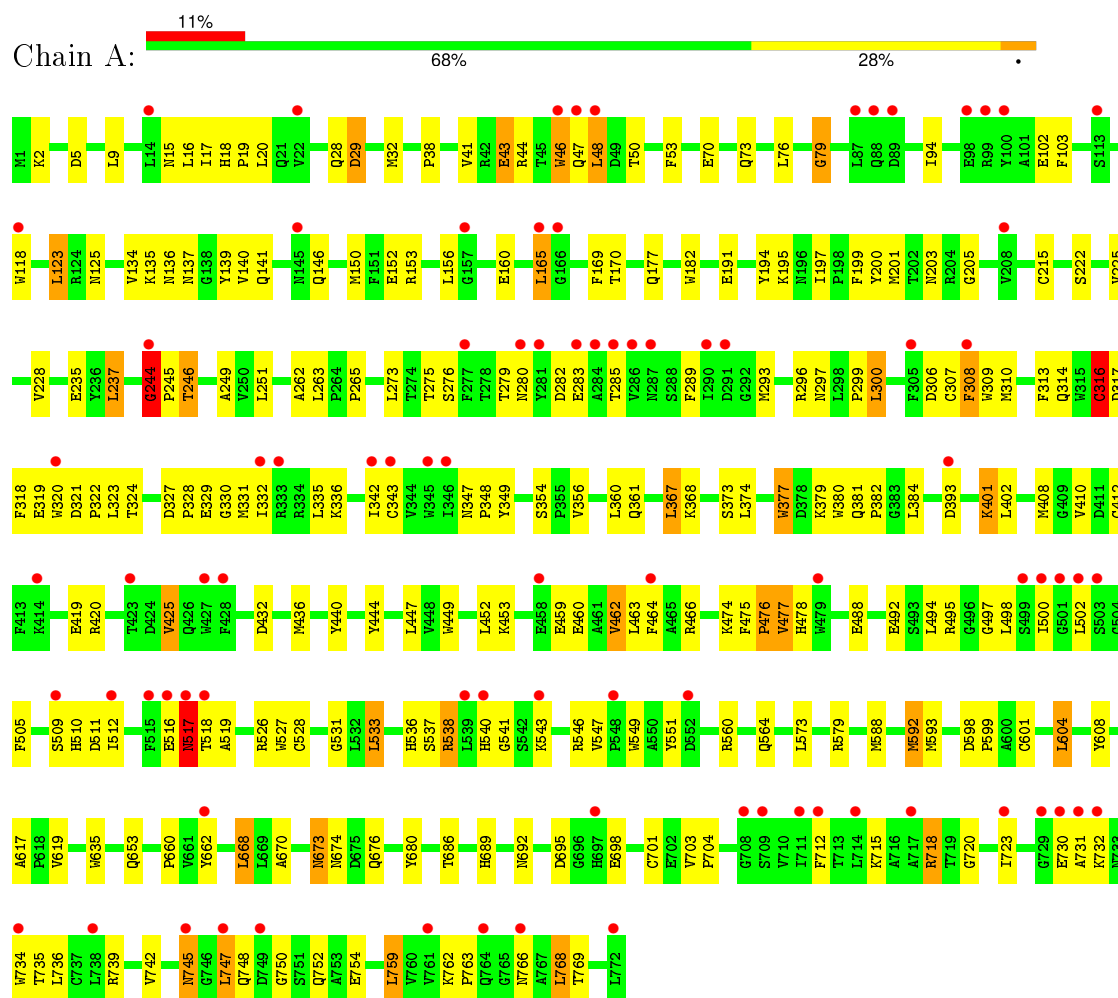
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	80	Total	O	0	0
			80	80		
3	C	108	Total	O	0	0
			108	108		
3	D	110	Total	O	0	0
			110	110		
3	E	61	Total	O	0	0
			61	61		
3	F	73	Total	O	0	0
			73	73		



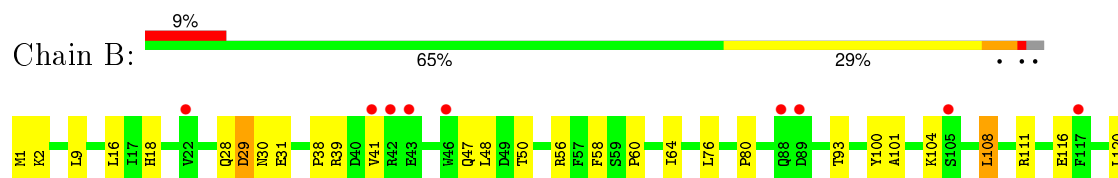
### 3 Residue-property plots

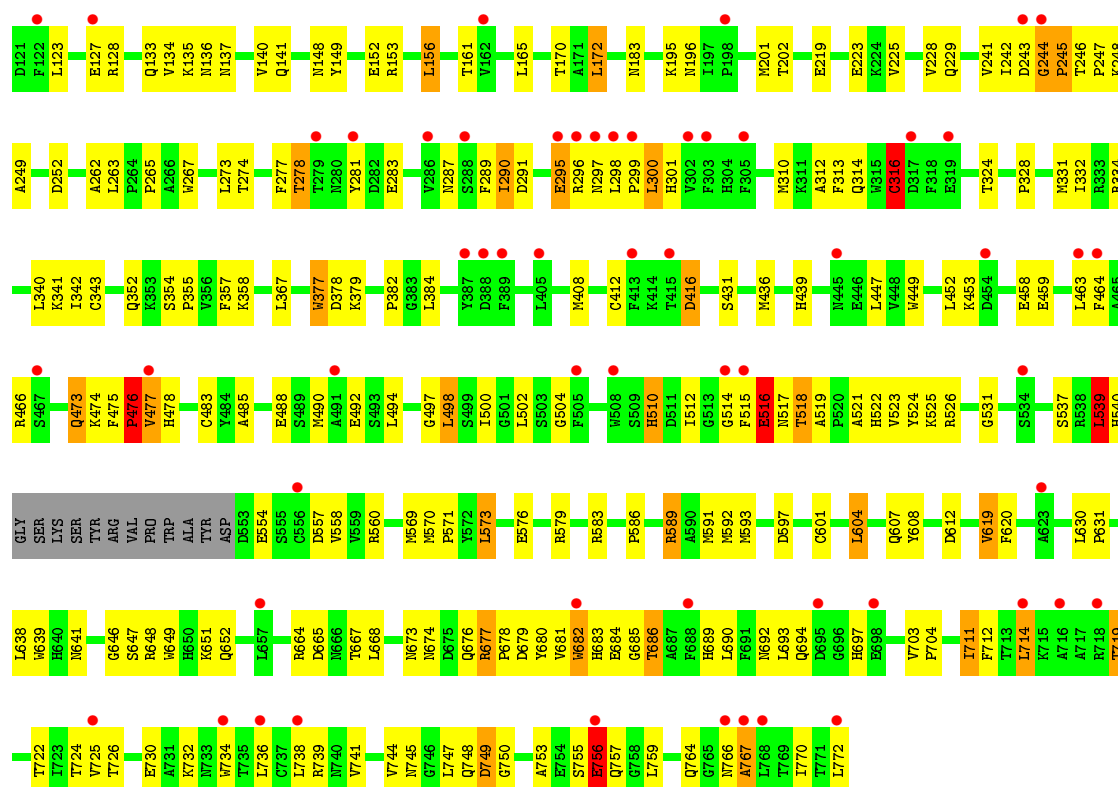
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Putative family 31 glucosidase yicI

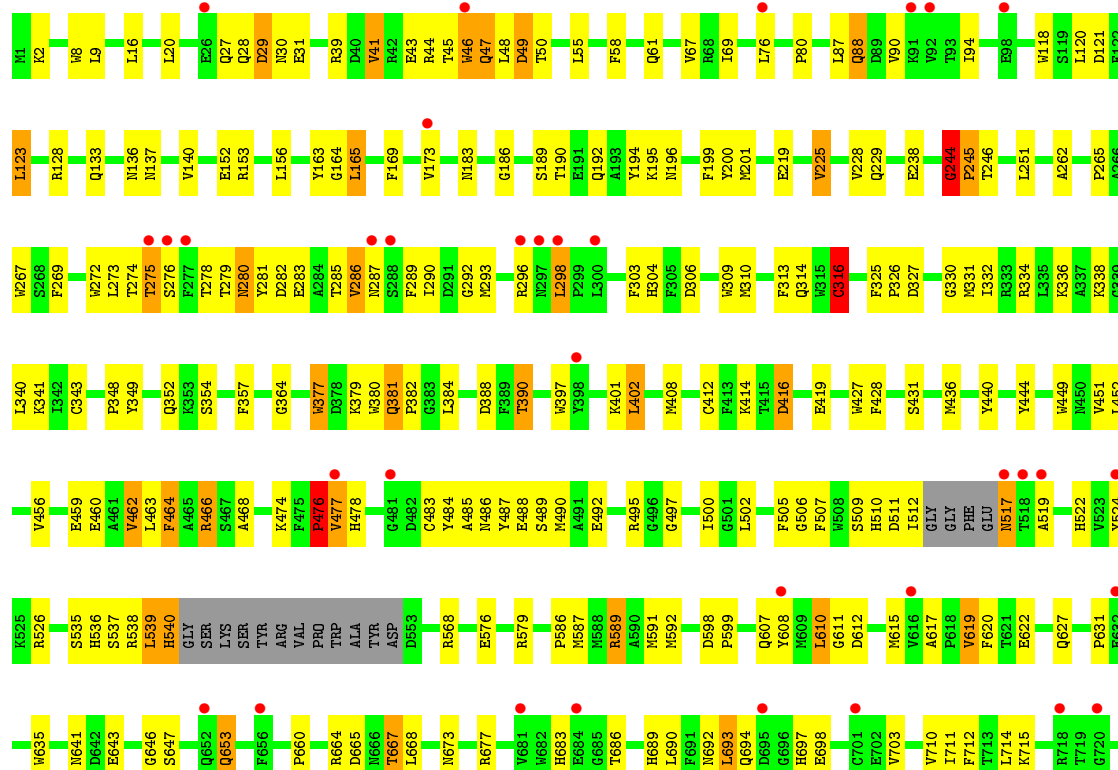


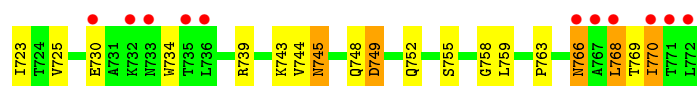
- Molecule 1: Putative family 31 glucosidase yicI



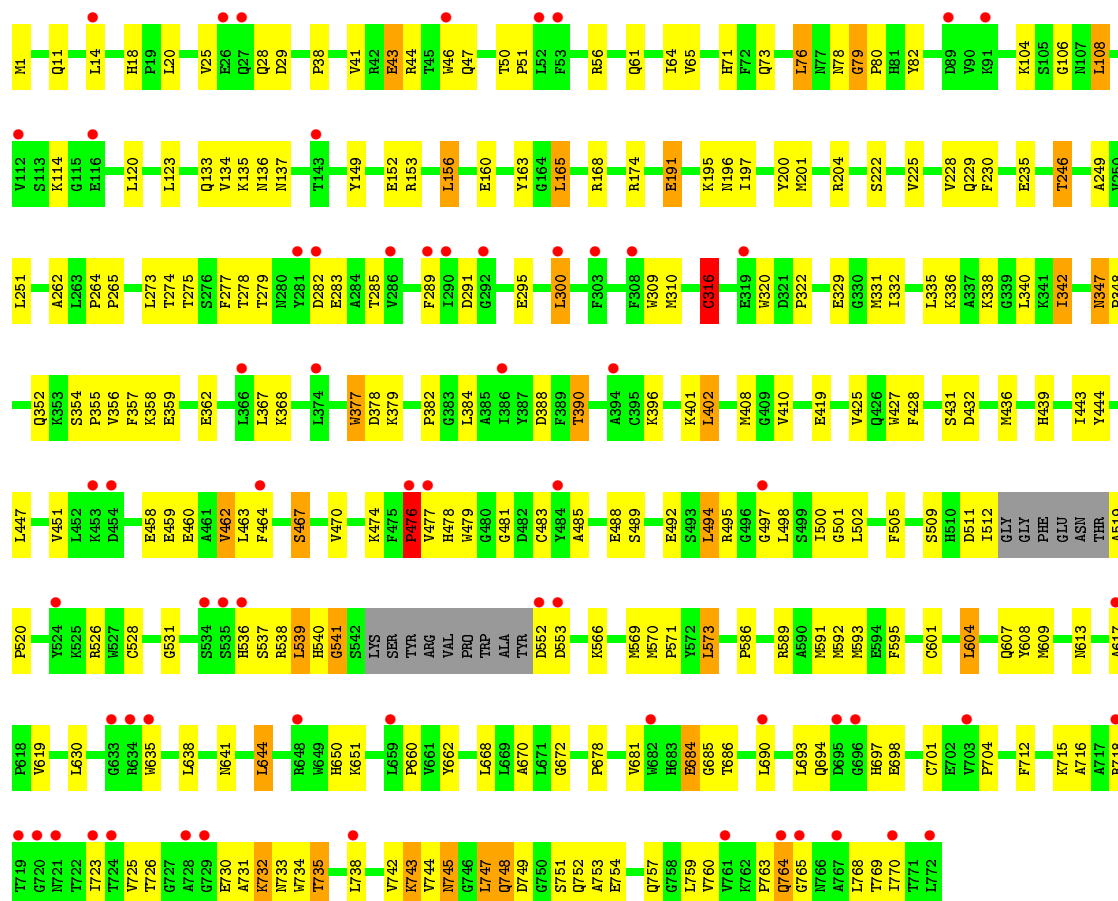


• Molecule 1: Putative family 31 glucosidase yicI

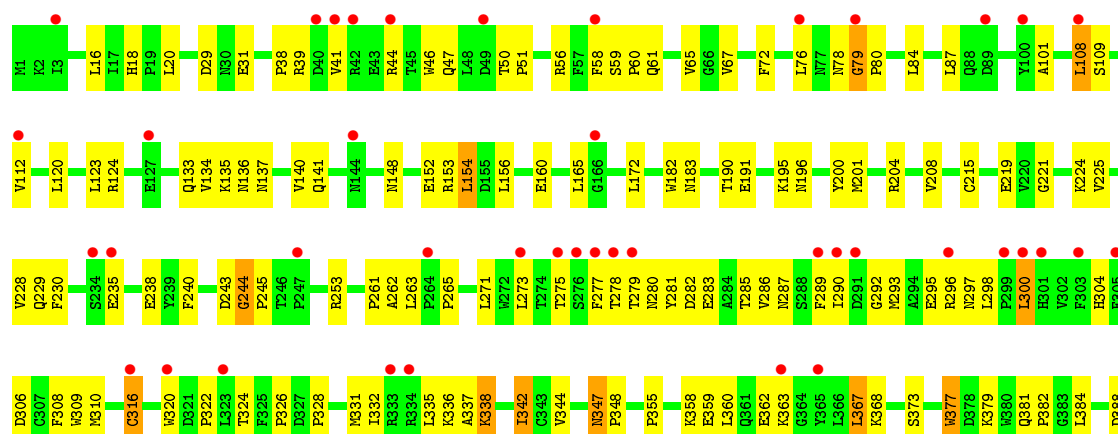


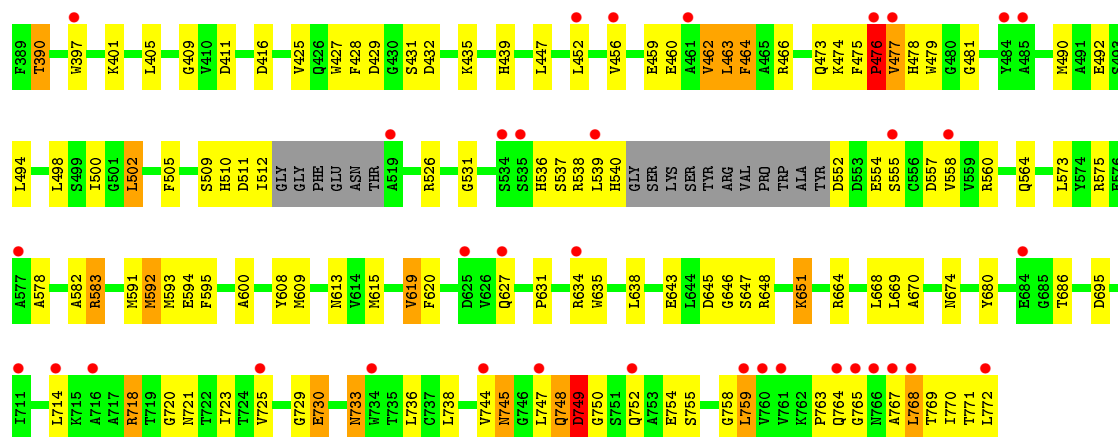


• Molecule 1: Putative family 31 glucosidase yicI

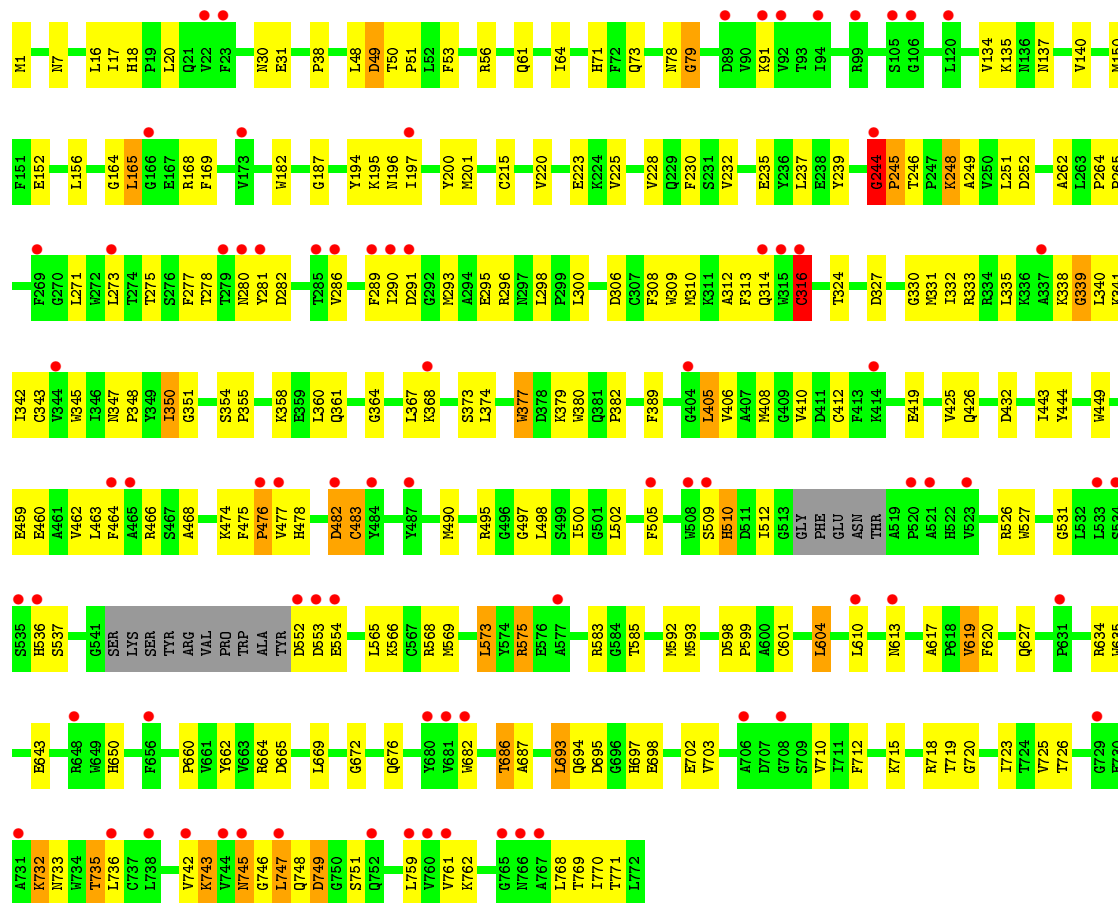


• Molecule 1: Putative family 31 glucosidase yicI





• Molecule 1: Putative family 31 glucosidase yicI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.34Å 174.79Å 209.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 39.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.40) 99.2 (39.61-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.247 0.210 , 0.201	Depositor DCC
$R_{free}$ test set	20672 reflections (9.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	5 of 228751 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	37302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: MES

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	0.38	0/6387	0.66	2/8650 (0.0%)
1	B	0.38	0/6280	0.66	4/8502 (0.0%)
1	C	0.40	0/6250	0.66	3/8461 (0.0%)
1	D	0.38	0/6253	0.66	3/8464 (0.0%)
1	E	0.38	0/6243	0.64	1/8451 (0.0%)
1	F	0.37	0/6251	0.64	1/8461 (0.0%)
All	All	0.38	0/37664	0.65	14/50989 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	CYS	CA-CB-SG	-6.30	102.66	114.00
1	C	316	CYS	CA-CB-SG	-6.12	102.99	114.00
1	C	416	ASP	N-CA-C	6.06	127.36	111.00
1	D	316	CYS	CA-CB-SG	-5.73	103.69	114.00
1	B	416	ASP	N-CA-C	5.69	126.36	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	6222	0	5932	236	0
1	B	6121	0	5839	225	0
1	C	6093	0	5817	231	0
1	D	6096	0	5816	202	0
1	E	6086	0	5808	230	0
1	F	6094	0	5814	192	0
2	A	12	0	13	1	0
2	B	12	0	13	0	0
2	C	12	0	13	2	0
2	D	12	0	13	0	0
2	E	12	0	13	1	0
2	F	12	0	13	0	0
3	A	86	0	0	1	0
3	B	80	0	0	3	0
3	C	108	0	0	3	0
3	D	110	0	0	2	0
3	E	61	0	0	1	0
3	F	73	0	0	1	0
All	All	37302	0	35104	1268	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 18.

The worst 5 of 1268 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:E:591:MSE:SE	1:E:609:MSE:HE3	1.99	1.12
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.21	1.11
1:B:591:MSE:HE3	1:B:607:GLN:HG3	1.32	1.11
1:D:591:MSE:HE3	1:D:607:GLN:HG3	1.34	1.10
1:A:310:MSE:HE1	1:A:317:ASP:H	1.08	1.09

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	770/772 (100%)	722 (94%)	39 (5%)	9 (1%)	16	23
1	B	756/772 (98%)	702 (93%)	40 (5%)	14 (2%)	10	12
1	C	750/772 (97%)	695 (93%)	46 (6%)	9 (1%)	16	23
1	D	751/772 (97%)	700 (93%)	39 (5%)	12 (2%)	12	16
1	E	749/772 (97%)	696 (93%)	45 (6%)	8 (1%)	17	25
1	F	751/772 (97%)	703 (94%)	38 (5%)	10 (1%)	15	21
All	All	4527/4632 (98%)	4218 (93%)	247 (6%)	62 (1%)	14	19

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ASP
1	B	539	LEU
1	B	749	ASP
1	B	767	ALA
1	C	29	ASP

### 5.3.2 Protein sidechains ⓘ

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	659/640 (103%)	613 (93%)	46 (7%)	19	29
1	B	649/640 (101%)	608 (94%)	41 (6%)	22	35
1	C	647/640 (101%)	602 (93%)	45 (7%)	19	29
1	D	647/640 (101%)	602 (93%)	45 (7%)	19	29
1	E	646/640 (101%)	605 (94%)	41 (6%)	22	35
1	F	646/640 (101%)	610 (94%)	36 (6%)	26	41
All	All	3894/3840 (101%)	3640 (94%)	254 (6%)	21	33

5 of 254 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	C	537	SER
1	D	300	LEU
1	F	464	PHE
1	C	610	LEU
1	C	749	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	GLN
1	C	733	ASN
1	F	107	ASN
1	C	146	GLN
1	C	522	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands 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
2	MES	A	801	-	11,12,12	0.58	0	14,16,16	0.98	2 (14%)
2	MES	B	802	-	11,12,12	0.51	0	14,16,16	0.84	1 (7%)
2	MES	C	803	-	11,12,12	0.44	0	14,16,16	0.80	0
2	MES	D	804	-	11,12,12	0.50	0	14,16,16	0.88	1 (7%)
2	MES	E	805	-	11,12,12	0.50	0	14,16,16	0.77	0
2	MES	F	806	-	11,12,12	0.43	0	14,16,16	1.37	2 (14%)

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
2	MES	A	801	-	-	0/6/14/14	0/1/1/1
2	MES	B	802	-	-	0/6/14/14	0/1/1/1
2	MES	C	803	-	-	0/6/14/14	0/1/1/1
2	MES	D	804	-	-	0/6/14/14	0/1/1/1
2	MES	E	805	-	-	0/6/14/14	0/1/1/1
2	MES	F	806	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	806	MES	O1S-S-C8	-3.86	103.61	106.91
2	D	804	MES	O1S-S-C8	-2.36	104.89	106.91
2	B	802	MES	O1S-S-C8	-2.32	104.93	106.91
2	A	801	MES	O1S-S-C8	-2.02	105.18	106.91
2	A	801	MES	O2S-S-C8	2.03	108.63	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	MES	1	0
2	C	803	MES	2	0
2	E	805	MES	1	0

## 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	753/772 (97%)	0.35	84 (11%) 7 7	29, 45, 79, 101	0
1	B	741/772 (95%)	0.39	66 (8%) 12 12	31, 45, 86, 102	0
1	C	737/772 (95%)	0.24	45 (6%) 25 25	30, 43, 75, 95	0
1	D	738/772 (95%)	0.25	64 (8%) 13 12	29, 42, 75, 100	0
1	E	736/772 (95%)	0.39	78 (10%) 8 8	31, 47, 79, 99	0
1	F	738/772 (95%)	0.46	78 (10%) 8 8	32, 48, 82, 100	0
All	All	4443/4632 (95%)	0.35	415 (9%) 11 10	29, 45, 79, 102	0

The worst 5 of 415 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	LEU	17.8
1	A	516	GLU	11.4
1	B	768	LEU	11.0
1	F	766	ASN	10.4
1	C	287	ASN	10.4

### 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	MES	B	802	12/12	0.91	0.27	1.05	81,85,86,87	0
2	MES	F	806	12/12	0.92	0.24	0.63	67,73,76,76	0
2	MES	A	801	12/12	0.85	0.30	0.60	81,82,83,83	0
2	MES	E	805	12/12	0.84	0.25	0.58	79,80,81,81	0
2	MES	C	803	12/12	0.84	0.24	0.20	54,59,60,62	0
2	MES	D	804	12/12	0.97	0.10	-1.03	56,64,67,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.