



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:46 PM GMT

PDB ID : 4MLG  
Title : Structure of RS223-Beta-xylosidase  
Authors : Jordan, D.; Braker, J.; Wagschal, K.; Lee, C.; Dubrovskaya, I.; Anderson, S.;  
Wawrzak, Z.  
Deposited on : 2013-09-06  
Resolution : 2.70 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](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.

---

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

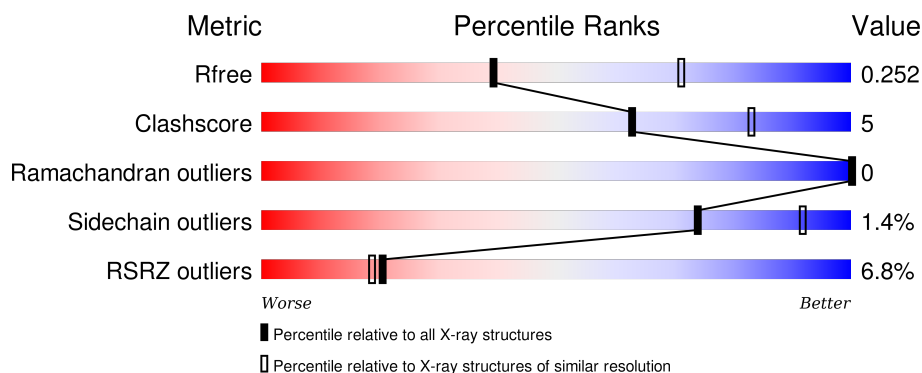
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	324	<div> <div>5%</div> <div>87%</div> <div>13%</div> </div>
1	B	324	<div> <div>4%</div> <div>86%</div> <div>13%</div> </div>
1	C	324	<div> <div>7%</div> <div>87%</div> <div>12%</div> </div>
1	D	324	<div> <div>2%</div> <div>84%</div> <div>16%</div> <div>•</div> </div>
1	E	324	<div> <div>6%</div> <div>85%</div> <div>15%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	324	
1	G	324	
1	H	324	
1	I	324	
1	J	324	
1	K	324	
1	L	324	

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	CA	A	401	-	-	-	X
2	CA	B	401	-	-	-	X
2	CA	C	401	-	-	-	X
2	CA	E	401	-	-	-	X
2	CA	F	401	-	-	-	X
2	CA	G	401	-	-	-	X
2	CA	H	401	-	-	-	X
2	CA	I	401	-	-	-	X
2	CA	J	401	-	-	-	X
2	CA	K	401	-	-	-	X
2	CA	L	401	-	-	-	X
3	SO4	A	402	-	-	-	X
3	SO4	C	403	-	-	-	X
3	SO4	D	402	-	-	-	X
3	SO4	D	403	-	-	-	X
3	SO4	E	402	-	-	-	X
3	SO4	F	402	-	-	-	X
3	SO4	F	403	-	-	-	X
3	SO4	G	402	-	-	-	X
3	SO4	G	403	-	-	-	X
3	SO4	H	403	-	-	-	X
3	SO4	I	402	-	-	-	X
3	SO4	I	403	-	-	-	X
3	SO4	J	403	-	-	-	X
3	SO4	K	402	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	K	403	-	-	-	X
3	SO4	L	403	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32402 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 Beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	B	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	C	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	D	322	Total	C	N	O	S	0	0	0
			2635	1696	437	487	15			
1	E	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	F	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	G	324	Total	C	N	O	S	0	0	0
			2641	1699	438	489	15			
1	H	324	Total	C	N	O	S	0	0	0
			2645	1701	438	491	15			
1	I	321	Total	C	N	O	S	0	0	0
			2615	1684	434	483	14			
1	J	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	K	324	Total	C	N	O	S	0	0	0
			2645	1701	438	491	15			
1	L	322	Total	C	N	O	S	0	0	0
			2631	1694	436	486	15			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

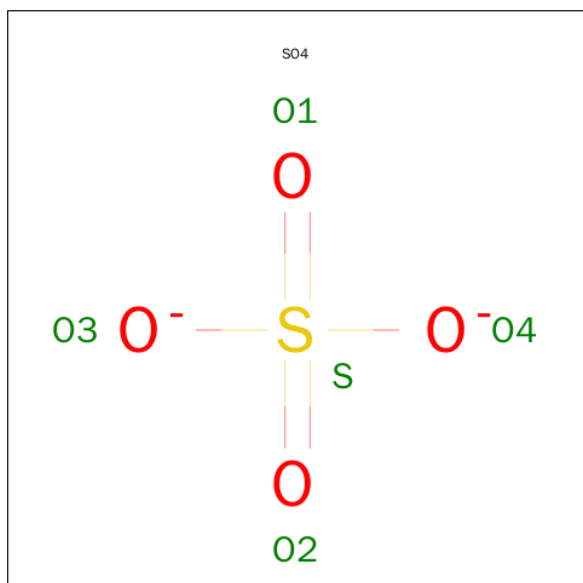
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		
2	K	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	I	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	L	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

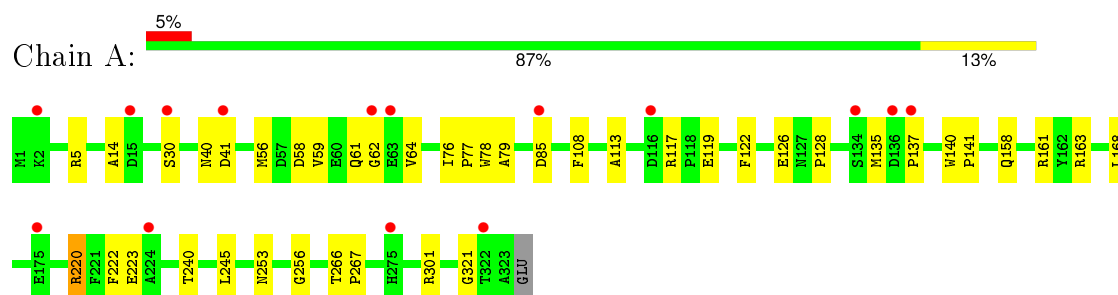
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	64	Total	O	0	0
			64	64		
4	C	45	Total	O	0	0
			45	45		
4	D	68	Total	O	0	0
			68	68		
4	E	50	Total	O	0	0
			50	50		
4	F	58	Total	O	0	0
			58	58		
4	G	47	Total	O	0	0
			47	47		
4	H	50	Total	O	0	0
			50	50		
4	I	49	Total	O	0	0
			49	49		
4	J	50	Total	O	0	0
			50	50		
4	K	44	Total	O	0	0
			44	44		
4	L	33	Total	O	0	0
			33	33		



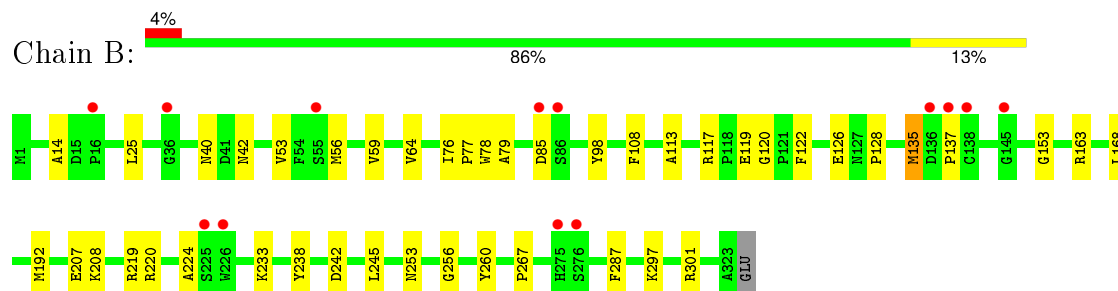
### 3 Residue-property plots [i](#)

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.

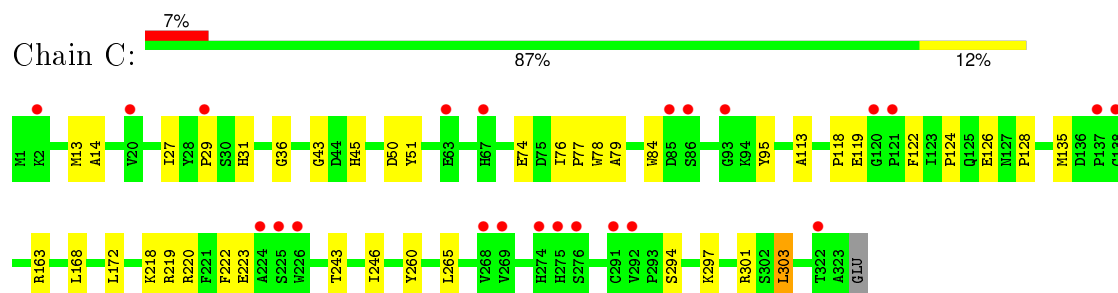
- Molecule 1: Beta-xylosidase



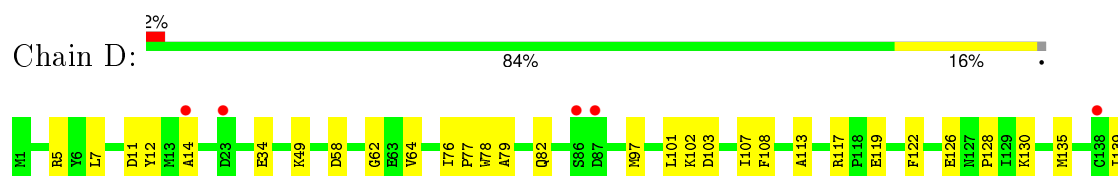
- Molecule 1: Beta-xylosidase

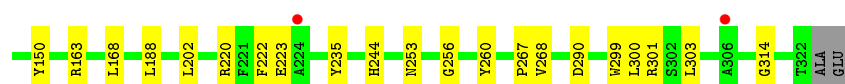


- Molecule 1: Beta-xylosidase

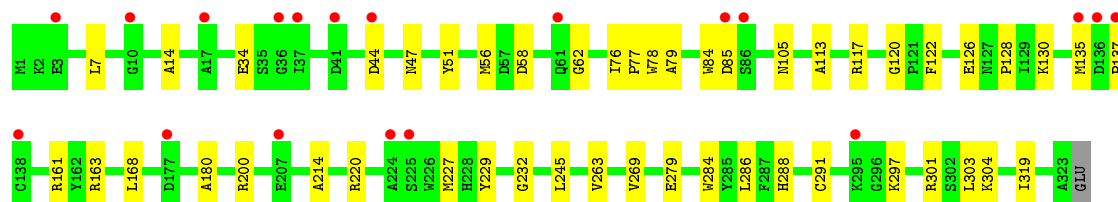
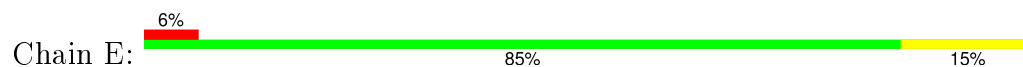


- Molecule 1: Beta-xylosidase

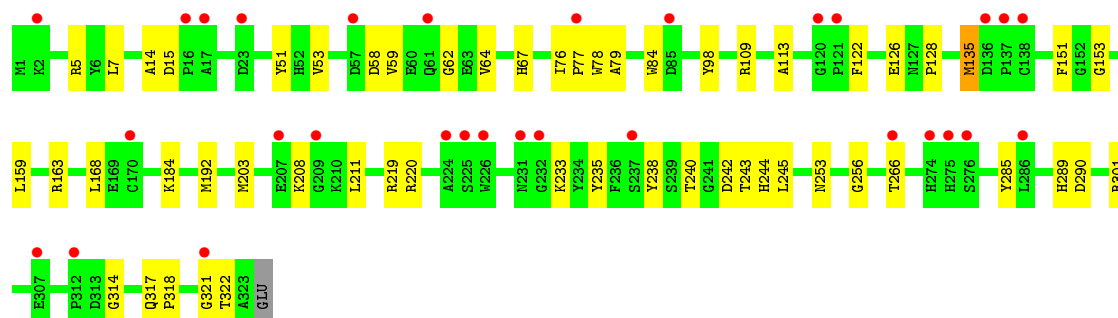
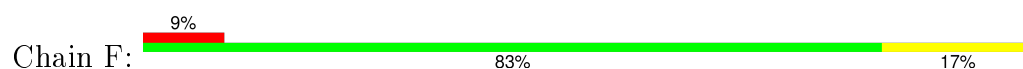




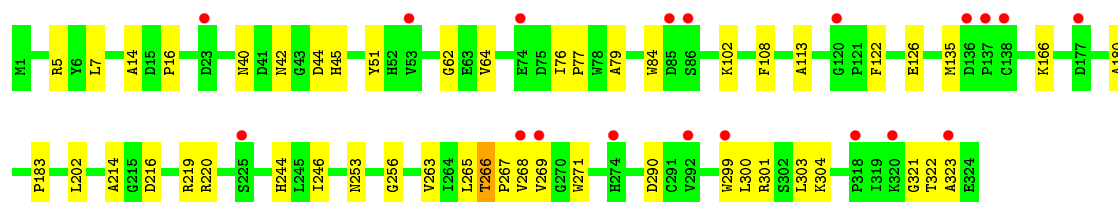
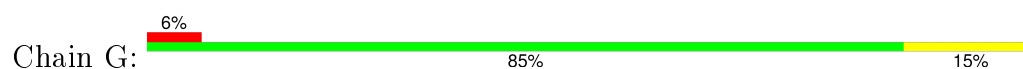
• Molecule 1: Beta-xylosidase



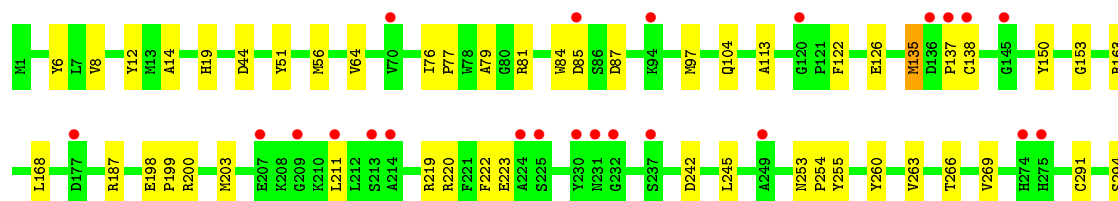
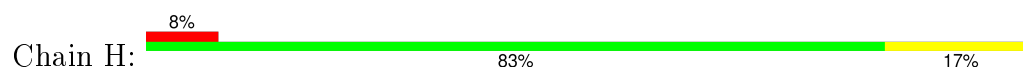
• Molecule 1: Beta-xylosidase

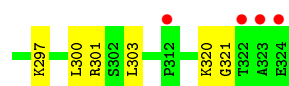


• Molecule 1: Beta-xylosidase

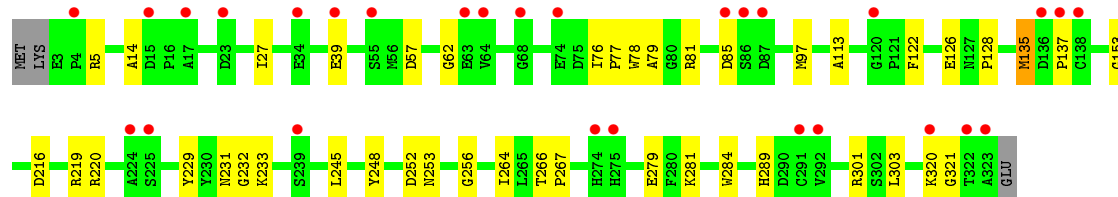
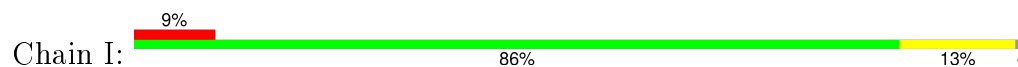


• Molecule 1: Beta-xylosidase

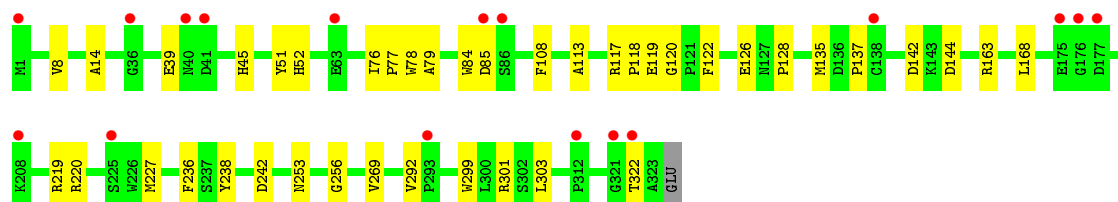
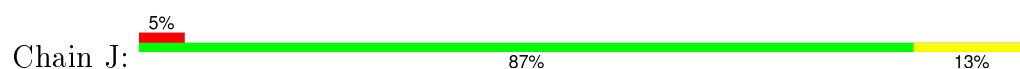




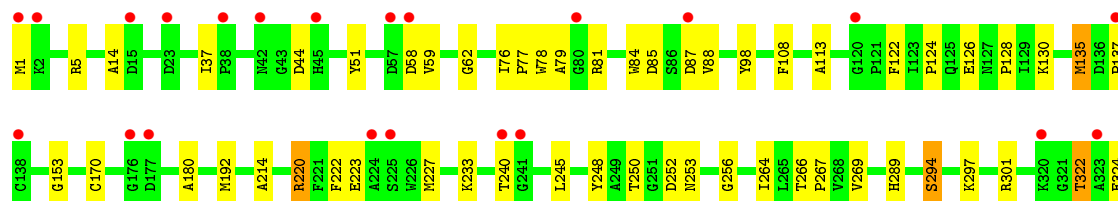
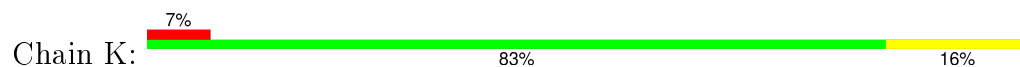
• Molecule 1: Beta-xylosidase



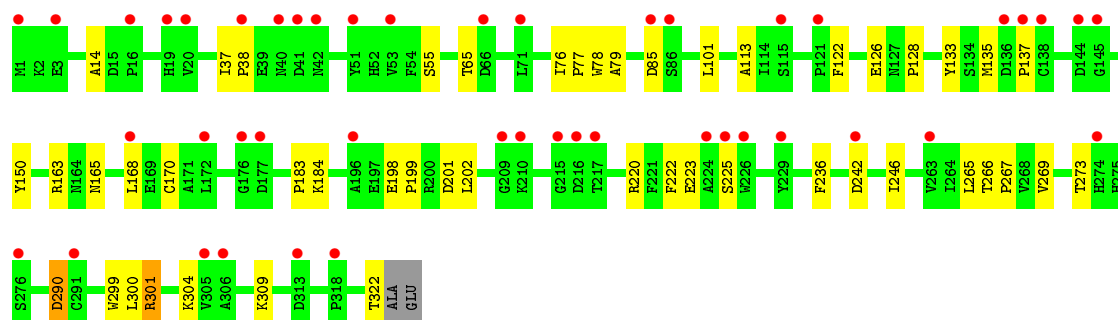
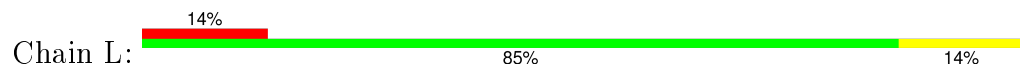
• Molecule 1: Beta-xylosidase



• Molecule 1: Beta-xylosidase



• Molecule 1: Beta-xylosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.53Å 148.70Å 125.65Å 90.00° 112.87° 90.00°	Depositor
Resolution (Å)	29.20 – 2.70 29.17 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.20-2.70) 91.8 (29.17-2.69)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.210 , 0.257 0.205 , 0.252	Depositor DCC
$R_{free}$ test set	5339 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 37.7	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 115104 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	0.22	0/2729	0.39	0/3706
1	B	0.22	0/2729	0.38	0/3706
1	C	0.21	0/2725	0.38	0/3702
1	D	0.22	0/2724	0.38	0/3699
1	E	0.22	0/2729	0.38	0/3706
1	F	0.23	0/2725	0.38	0/3702
1	G	0.21	0/2730	0.37	0/3709
1	H	0.22	0/2734	0.39	0/3714
1	I	0.21	0/2704	0.37	0/3675
1	J	0.22	0/2725	0.38	0/3702
1	K	0.22	0/2734	0.38	0/3714
1	L	0.21	0/2720	0.37	0/3694
All	All	0.22	0/32708	0.38	0/44429

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

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	2640	0	2490	20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2640	0	2490	21	0
1	C	2636	0	2479	25	0
1	D	2635	0	2485	26	0
1	E	2640	0	2490	28	0
1	F	2636	0	2479	41	0
1	G	2641	0	2481	34	0
1	H	2645	0	2485	30	0
1	I	2615	0	2455	26	0
1	J	2636	0	2479	27	0
1	K	2645	0	2485	30	0
1	L	2631	0	2479	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
3	I	10	0	0	0	0
3	J	10	0	0	0	0
3	K	10	0	0	0	0
3	L	10	0	0	0	0
4	A	72	0	0	0	0
4	B	64	0	0	0	0
4	C	45	0	0	0	0
4	D	68	0	0	0	0
4	E	50	0	0	2	0
4	F	58	0	0	0	0
4	G	47	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	50	0	0	2	0
4	I	49	0	0	1	0
4	J	50	0	0	1	0
4	K	44	0	0	1	0
4	L	33	0	0	0	0
All	All	32402	0	29777	328	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 5.

All (328) 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:G:265:LEU:HD12	1:G:266:THR:H	1.21	1.05
1:F:240:THR:CG2	1:F:243:THR:HB	2.13	0.79
1:G:265:LEU:HD12	1:G:266:THR:N	1.98	0.78
1:F:240:THR:HG22	1:F:243:THR:HB	1.69	0.74
1:L:266:THR:HG23	1:L:267:PRO:HD2	1.70	0.72
1:H:104:GLN:HG3	4:H:507:HOH:O	1.90	0.71
1:J:118:PRO:HG2	1:J:119:GLU:OE1	1.89	0.71
1:F:243:THR:HG22	1:F:245:LEU:HG	1.75	0.67
1:A:220:ARG:NH2	1:A:240:THR:O	2.28	0.67
1:G:290:ASP:HB2	1:G:304:LYS:HD2	1.75	0.66
1:G:76:ILE:HB	1:G:79:ALA:HB2	1.76	0.66
1:E:77:PRO:HG2	1:E:126:GLU:HA	1.78	0.66
1:K:76:ILE:HB	1:K:79:ALA:HB2	1.78	0.66
1:C:76:ILE:HB	1:C:79:ALA:HB2	1.78	0.66
1:J:76:ILE:HB	1:J:79:ALA:HB2	1.78	0.65
1:H:203:MET:HB2	1:H:211:LEU:HD21	1.79	0.64
1:E:269:VAL:HG23	1:E:291:CYS:H	1.62	0.64
1:I:77:PRO:HG2	1:I:126:GLU:HA	1.80	0.64
1:E:44:ASP:O	1:E:47:ASN:ND2	2.32	0.62
1:H:76:ILE:HB	1:H:79:ALA:HB2	1.80	0.62
1:F:76:ILE:HB	1:F:79:ALA:HB2	1.81	0.62
1:B:253:ASN:HD21	1:B:256:GLY:HA3	1.65	0.62
1:E:117:ARG:HG3	1:E:120:GLY:H	1.66	0.61
1:I:57:ASP:O	1:I:281:LYS:NZ	2.33	0.61
1:G:246:ILE:HB	1:G:265:LEU:HB3	1.82	0.61
1:L:266:THR:CG2	1:L:267:PRO:HD2	2.30	0.61
1:L:76:ILE:HB	1:L:79:ALA:HB2	1.83	0.61
1:L:77:PRO:HG2	1:L:126:GLU:HA	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ALA:HB2	1:E:301:ARG:HB2	1.83	0.61
1:H:320:LYS:NZ	4:H:535:HOH:O	2.34	0.61
1:K:14:ALA:HB2	1:K:301:ARG:HB2	1.83	0.60
1:K:294:SER:HB3	1:K:297:LYS:HB2	1.84	0.60
1:I:113:ALA:HB1	1:I:122:PHE:HB3	1.82	0.60
1:K:269:VAL:HG23	1:K:322:THR:HB	1.85	0.59
1:F:240:THR:HG22	1:F:240:THR:O	2.03	0.59
1:B:14:ALA:HB2	1:B:301:ARG:HB2	1.85	0.59
1:A:76:ILE:HB	1:A:79:ALA:HB2	1.84	0.59
1:J:52:HIS:NE2	4:J:510:HOH:O	2.32	0.59
1:F:113:ALA:HB1	1:F:122:PHE:HB3	1.85	0.59
1:C:95:TYR:CZ	1:C:118:PRO:HG3	2.38	0.58
1:A:14:ALA:HB2	1:A:301:ARG:HB2	1.85	0.58
1:C:51:TYR:OH	1:C:84:TRP:O	2.20	0.58
1:J:117:ARG:HB3	1:J:119:GLU:OE2	2.03	0.58
1:E:7:LEU:HD13	1:E:56:MET:CE	2.34	0.58
1:C:77:PRO:HG2	1:C:126:GLU:HA	1.86	0.58
1:J:77:PRO:HG2	1:J:126:GLU:HA	1.86	0.58
1:F:14:ALA:HB2	1:F:301:ARG:HB2	1.86	0.58
1:H:297:LYS:HD2	1:H:300:LEU:HD12	1.86	0.58
1:D:7:LEU:HB3	1:D:64:VAL:HG21	1.86	0.57
1:B:77:PRO:HG2	1:B:126:GLU:HA	1.86	0.57
1:C:113:ALA:HB1	1:C:122:PHE:HB3	1.87	0.57
1:F:243:THR:HG21	1:F:245:LEU:HD12	1.86	0.56
1:L:113:ALA:HB1	1:L:122:PHE:HB3	1.87	0.56
1:G:113:ALA:HB1	1:G:122:PHE:HB3	1.87	0.56
1:D:103:ASP:OD1	1:D:107:ILE:N	2.33	0.56
1:E:7:LEU:HD12	1:E:303:LEU:CD1	2.35	0.56
1:L:37:ILE:HD12	1:L:38:PRO:HD2	1.88	0.56
1:F:266:THR:OG1	1:F:321:GLY:N	2.37	0.56
1:F:5:ARG:NH1	1:F:59:VAL:O	2.38	0.56
1:J:14:ALA:HB2	1:J:301:ARG:HB2	1.88	0.55
1:K:220:ARG:NH2	1:K:240:THR:O	2.38	0.55
1:B:207:GLU:HG2	1:B:208:LYS:HD2	1.88	0.55
1:C:14:ALA:HB2	1:C:301:ARG:HB2	1.88	0.55
1:L:290:ASP:HB2	1:L:304:LYS:HD2	1.88	0.55
1:L:133:TYR:OH	1:L:165:ASN:ND2	2.39	0.55
1:F:243:THR:CG2	1:F:245:LEU:HG	2.36	0.55
1:I:81:ARG:NH1	4:I:508:HOH:O	2.39	0.55
1:L:14:ALA:HB2	1:L:301:ARG:HB2	1.89	0.54
1:I:248:TYR:HB3	1:I:264:ILE:HD11	1.89	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ASN:ND2	1:D:256:GLY:H	2.07	0.53
1:D:76:ILE:HB	1:D:79:ALA:HB2	1.90	0.53
1:E:163:ARG:HG2	1:E:168:LEU:HD11	1.89	0.53
1:G:102:LYS:NZ	4:G:513:HOH:O	2.41	0.53
1:D:5:ARG:NH2	1:D:62:GLY:O	2.36	0.53
1:F:203:MET:HB3	1:F:211:LEU:HD21	1.91	0.53
1:F:242:ASP:OD1	1:F:242:ASP:N	2.42	0.53
1:I:97:MET:HB3	1:I:113:ALA:HB3	1.91	0.53
1:I:289:HIS:CE1	1:I:301:ARG:HD2	2.44	0.53
1:K:252:ASP:OD1	1:K:253:ASN:ND2	2.37	0.52
1:J:253:ASN:OD1	1:J:256:GLY:N	2.40	0.52
1:E:7:LEU:HD13	1:E:56:MET:HE2	1.90	0.52
1:H:14:ALA:HB2	1:H:301:ARG:HB2	1.92	0.52
1:H:8:VAL:HG23	1:H:303:LEU:HD11	1.92	0.52
1:A:253:ASN:HD21	1:A:256:GLY:HA3	1.74	0.52
1:K:113:ALA:HB1	1:K:122:PHE:HB3	1.91	0.52
1:G:263:VAL:HG13	1:G:265:LEU:O	2.10	0.52
1:E:200:ARG:NH2	4:E:530:HOH:O	2.43	0.52
1:F:15:ASP:H	1:F:289:HIS:CD2	2.28	0.51
1:B:219:ARG:HG2	1:B:260:TYR:CZ	2.45	0.51
1:J:113:ALA:HB1	1:J:122:PHE:HB3	1.92	0.51
1:I:5:ARG:NH2	1:I:62:GLY:O	2.29	0.51
1:H:113:ALA:HB1	1:H:122:PHE:HB3	1.92	0.51
1:F:242:ASP:O	1:F:244:HIS:NE2	2.43	0.51
1:J:51:TYR:OH	1:J:84:TRP:O	2.23	0.51
1:H:51:TYR:OH	1:H:84:TRP:O	2.21	0.51
1:G:268:VAL:HG13	1:G:290:ASP:OD1	2.11	0.51
1:I:14:ALA:HB2	1:I:301:ARG:HB2	1.92	0.51
1:L:55:SER:HB3	1:L:65:THR:HB	1.93	0.50
1:K:1:MET:HG2	1:K:1:MET:O	2.11	0.50
1:D:113:ALA:HB1	1:D:122:PHE:HB3	1.94	0.50
1:G:77:PRO:HG2	1:G:126:GLU:HA	1.93	0.50
1:F:289:HIS:CE1	1:F:301:ARG:HD2	2.47	0.50
1:G:267:PRO:HB2	1:G:323:ALA:O	2.12	0.50
1:E:76:ILE:HB	1:E:79:ALA:HB2	1.93	0.50
1:L:273:THR:O	1:L:273:THR:HG23	2.11	0.50
1:K:77:PRO:HG2	1:K:126:GLU:HA	1.93	0.50
1:B:53:VAL:HG11	1:B:119:GLU:HA	1.94	0.50
1:A:77:PRO:HG2	1:A:126:GLU:HA	1.94	0.49
1:J:8:VAL:HG23	1:J:303:LEU:HD11	1.94	0.49
1:K:180:ALA:HB2	1:K:214:ALA:HA	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:ASN:OD1	1:K:256:GLY:N	2.42	0.49
1:D:97:MET:HB3	1:D:113:ALA:HB3	1.94	0.49
1:I:252:ASP:OD1	1:I:253:ASN:ND2	2.37	0.49
1:D:163:ARG:HG2	1:D:168:LEU:HD11	1.94	0.49
1:D:82:GLN:OE1	1:D:102:LYS:HD2	2.12	0.49
1:C:74:GLU:N	1:C:74:GLU:OE2	2.46	0.49
1:H:242:ASP:N	1:H:242:ASP:OD1	2.43	0.49
1:J:78:TRP:CG	1:J:128:PRO:HD3	2.48	0.49
1:L:183:PRO:HG2	1:L:202:LEU:HB3	1.95	0.49
1:E:279:GLU:HB2	1:E:284:TRP:CE2	2.48	0.49
1:D:14:ALA:HB2	1:D:301:ARG:HB2	1.95	0.48
1:H:77:PRO:HG2	1:H:126:GLU:HA	1.94	0.48
1:E:34:GLU:OE1	1:E:297:LYS:NZ	2.29	0.48
1:I:216:ASP:OD2	1:I:219:ARG:NH1	2.45	0.48
1:I:253:ASN:HD21	1:I:256:GLY:HA3	1.79	0.48
1:F:135:MET:SD	1:F:153:GLY:HA3	2.54	0.48
1:F:77:PRO:HG2	1:F:126:GLU:HA	1.95	0.48
1:A:56:MET:HE3	1:A:64:VAL:HG22	1.95	0.48
1:C:119:GLU:N	1:C:119:GLU:OE1	2.43	0.48
1:C:27:ILE:HG22	1:C:29:PRO:HD3	1.95	0.48
1:L:299:TRP:CD1	1:L:300:LEU:HG	2.48	0.48
1:J:269:VAL:HG23	1:J:322:THR:HB	1.96	0.48
1:K:58:ASP:HB3	1:K:62:GLY:HA3	1.95	0.48
1:L:225:SER:HG	1:L:236:PHE:HE1	1.62	0.48
1:A:117:ARG:NH1	1:A:119:GLU:OE2	2.46	0.48
1:H:163:ARG:HG2	1:H:168:LEU:HD11	1.95	0.48
1:K:248:TYR:HB3	1:K:264:ILE:HD11	1.96	0.48
1:K:170:CYS:HA	1:L:170:CYS:HA	1.96	0.48
1:G:253:ASN:ND2	1:G:256:GLY:H	2.12	0.48
1:F:98:TYR:OH	1:F:192:MET:HB3	2.13	0.47
1:K:245:LEU:HD23	1:K:267:PRO:HD3	1.95	0.47
1:C:36:GLY:HA3	1:H:6:TYR:O	2.14	0.47
1:G:14:ALA:HB2	1:G:301:ARG:HB2	1.95	0.47
1:J:85:ASP:O	1:J:137:PRO:HD2	2.15	0.47
1:E:113:ALA:HB1	1:E:122:PHE:HB3	1.96	0.47
1:F:253:ASN:HD21	1:F:256:GLY:HA3	1.79	0.47
1:F:163:ARG:HG2	1:F:168:LEU:HD11	1.97	0.47
1:D:117:ARG:NH2	1:D:119:GLU:OE2	2.47	0.47
1:B:56:MET:SD	1:B:64:VAL:HG22	2.53	0.47
1:L:85:ASP:O	1:L:137:PRO:HD2	2.15	0.47
1:J:45:HIS:HD2	1:J:299:TRP:HB3	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:GLY:O	1:F:159:LEU:HB2	2.14	0.47
1:C:163:ARG:HG2	1:C:168:LEU:HD11	1.96	0.47
1:G:265:LEU:CD1	1:G:266:THR:H	2.08	0.47
1:A:5:ARG:NH1	1:A:59:VAL:O	2.46	0.47
1:G:303:LEU:N	4:G:508:HOH:O	2.37	0.47
1:I:266:THR:HG1	1:I:321:GLY:H	1.59	0.47
1:G:263:VAL:O	1:G:263:VAL:HG12	2.13	0.47
1:F:290:ASP:OD2	1:F:322:THR:HG21	2.15	0.47
1:A:113:ALA:HB1	1:A:122:PHE:HB3	1.95	0.47
1:K:233:LYS:HD2	1:K:250:THR:HG23	1.97	0.46
1:G:265:LEU:CD1	1:G:266:THR:N	2.73	0.46
1:F:233:LYS:HE2	1:F:314:GLY:HA3	1.98	0.46
1:G:42:ASN:ND2	1:G:44:ASP:OD2	2.48	0.46
1:I:39:GLU:O	1:I:39:GLU:HG3	2.15	0.46
1:H:138:CYS:SG	1:H:150:TYR:HB2	2.56	0.46
1:H:97:MET:HB3	1:H:113:ALA:HB3	1.98	0.46
1:G:40:ASN:H	1:G:45:HIS:CD2	2.33	0.46
1:K:85:ASP:O	1:K:137:PRO:HD2	2.15	0.46
1:D:34:GLU:OE1	1:D:299:TRP:NE1	2.34	0.46
1:G:266:THR:OG1	1:G:321:GLY:N	2.48	0.46
1:J:117:ARG:HB2	1:J:120:GLY:H	1.81	0.46
1:A:266:THR:HG1	1:A:321:GLY:H	1.57	0.46
1:G:266:THR:HB	1:G:267:PRO:CD	2.46	0.46
1:B:245:LEU:HD23	1:B:267:PRO:HD3	1.98	0.46
1:C:246:ILE:HB	1:C:265:LEU:HB3	1.98	0.46
1:A:14:ALA:O	1:A:30:SER:N	2.45	0.46
1:E:58:ASP:HB3	1:E:62:GLY:HA3	1.98	0.46
1:C:31:HIS:ND1	1:C:50:ASP:OD1	2.46	0.46
1:E:105:ASN:OD1	1:F:109:ARG:NH1	2.46	0.45
1:K:135:MET:SD	1:K:153:GLY:HA3	2.56	0.45
1:C:218:LYS:HG2	1:C:243:THR:HG21	1.98	0.45
1:G:5:ARG:NH2	1:G:62:GLY:O	2.39	0.45
1:L:246:ILE:HB	1:L:265:LEU:HB3	1.98	0.45
1:H:187:ARG:HB2	1:H:255:TYR:OH	2.16	0.45
1:H:222:PHE:HD2	1:H:223:GLU:HG2	1.82	0.45
1:F:7:LEU:HB3	1:F:64:VAL:HG21	1.98	0.45
1:L:222:PHE:HD2	1:L:223:GLU:HG2	1.82	0.45
1:B:25:LEU:HD22	1:B:59:VAL:HG22	1.97	0.45
1:F:53:VAL:HG13	1:F:67:HIS:HB2	1.98	0.45
1:F:242:ASP:O	1:F:244:HIS:CD2	2.70	0.45
1:C:222:PHE:HD2	1:C:223:GLU:HG2	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:O	1:A:137:PRO:HD2	2.16	0.45
1:C:78:TRP:CG	1:C:128:PRO:HD3	2.53	0.44
1:F:51:TYR:OH	1:F:84:TRP:O	2.28	0.44
1:A:245:LEU:HD23	1:A:267:PRO:HD3	1.99	0.44
1:C:219:ARG:HG2	1:C:260:TYR:CZ	2.52	0.44
1:D:222:PHE:HD2	1:D:223:GLU:HG2	1.82	0.44
1:F:78:TRP:CG	1:F:128:PRO:HD3	2.52	0.44
1:H:266:THR:HG1	1:H:321:GLY:H	1.61	0.44
1:G:45:HIS:CD2	1:G:45:HIS:H	2.34	0.44
1:G:51:TYR:OH	1:G:84:TRP:O	2.25	0.44
1:L:242:ASP:OD1	1:L:242:ASP:N	2.48	0.44
1:F:151:PHE:CE1	1:F:184:LYS:HB2	2.53	0.44
1:D:268:VAL:HB	1:D:290:ASP:HB3	1.99	0.44
1:H:19:HIS:NE2	1:H:87:ASP:OD1	2.40	0.44
1:H:135:MET:SD	1:H:153:GLY:HA3	2.58	0.44
1:F:317:GLN:HA	1:F:318:PRO:HD3	1.89	0.44
1:J:253:ASN:HD21	1:J:256:GLY:HA3	1.82	0.44
1:D:260:TYR:O	1:E:117:ARG:NH1	2.44	0.44
1:K:5:ARG:NH1	1:K:59:VAL:O	2.43	0.44
1:C:95:TYR:CE1	1:C:118:PRO:HG3	2.53	0.43
1:H:56:MET:HE3	1:H:64:VAL:HG22	1.99	0.43
1:I:135:MET:SD	1:I:153:GLY:HA3	2.58	0.43
1:J:39:GLU:HG3	1:J:45:HIS:CE1	2.53	0.43
1:J:227:MET:HE1	1:J:236:PHE:HB2	2.00	0.43
1:H:219:ARG:HG2	1:H:260:TYR:CZ	2.53	0.43
1:J:219:ARG:O	1:J:238:TYR:OH	2.30	0.43
1:L:184:LYS:NZ	1:L:201:ASP:OD1	2.35	0.43
1:B:40:ASN:ND2	1:B:42:ASN:OD1	2.50	0.43
1:F:151:PHE:CZ	1:F:184:LYS:HB2	2.53	0.43
1:G:244:HIS:ND1	1:G:271:TRP:O	2.44	0.43
1:J:292:VAL:HG21	1:J:322:THR:HG21	1.99	0.43
1:C:78:TRP:HA	1:D:130:LYS:HD3	2.00	0.43
1:H:44:ASP:OD1	1:H:81:ARG:NH1	2.40	0.43
1:B:113:ALA:HB1	1:B:122:PHE:HB3	1.99	0.43
1:I:245:LEU:HD23	1:I:267:PRO:HD3	2.00	0.43
1:D:139:ILE:HD12	1:D:188:LEU:HD11	2.00	0.43
1:K:130:LYS:NZ	4:K:511:HOH:O	2.45	0.43
1:G:7:LEU:HB3	1:G:64:VAL:HG21	2.01	0.43
1:J:117:ARG:NE	1:J:119:GLU:OE2	2.52	0.43
1:L:79:ALA:HA	1:L:101:LEU:HD21	2.01	0.43
1:D:103:ASP:OD1	1:D:107:ILE:O	2.37	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ASP:HB3	1:J:144:ASP:OD1	2.19	0.43
1:G:269:VAL:H	1:G:322:THR:HB	1.84	0.43
1:J:119:GLU:CD	1:J:119:GLU:H	2.22	0.43
1:E:78:TRP:CG	1:E:128:PRO:HD3	2.54	0.43
1:B:78:TRP:CG	1:B:128:PRO:HD3	2.54	0.43
1:C:43:GLY:HA2	1:C:45:HIS:CE1	2.53	0.42
1:E:161:ARG:NH2	4:E:533:HOH:O	2.52	0.42
1:F:240:THR:HG21	1:F:243:THR:HB	1.99	0.42
1:D:77:PRO:HG2	1:D:126:GLU:HA	2.00	0.42
1:G:266:THR:HB	1:G:267:PRO:HD2	2.01	0.42
1:J:119:GLU:CD	1:J:119:GLU:N	2.73	0.42
1:H:253:ASN:HB2	1:H:254:PRO:HD2	2.01	0.42
1:E:85:ASP:O	1:E:137:PRO:HD2	2.20	0.42
1:D:58:ASP:HB3	1:D:62:GLY:HA3	2.01	0.42
1:A:58:ASP:O	1:A:62:GLY:HA3	2.19	0.42
1:B:242:ASP:N	1:B:242:ASP:OD1	2.51	0.42
1:C:294:SER:HB3	1:C:297:LYS:HB2	2.01	0.42
1:G:180:ALA:HB2	1:G:214:ALA:HA	2.01	0.42
1:K:113:ALA:HA	1:K:124:PRO:HA	2.02	0.42
1:B:135:MET:SD	1:B:153:GLY:HA3	2.59	0.42
1:D:78:TRP:CG	1:D:128:PRO:HD3	2.55	0.42
1:H:269:VAL:O	1:H:291:CYS:N	2.49	0.42
1:K:222:PHE:HD2	1:K:223:GLU:HG2	1.84	0.42
1:K:44:ASP:OD1	1:K:81:ARG:NH1	2.52	0.42
1:G:216:ASP:OD2	1:G:219:ARG:HD3	2.18	0.42
1:G:166:LYS:NZ	1:H:104:GLN:O	2.36	0.42
1:D:78:TRP:CH2	1:D:101:LEU:HB3	2.54	0.42
1:E:286:LEU:HD22	1:E:319:ILE:HD12	2.02	0.42
1:I:233:LYS:HB2	1:I:233:LYS:HE3	1.90	0.42
1:I:85:ASP:O	1:I:137:PRO:HD2	2.19	0.42
1:E:51:TYR:OH	1:E:84:TRP:O	2.22	0.42
1:E:245:LEU:HD22	1:E:263:VAL:HG11	2.01	0.42
1:J:76:ILE:HA	1:J:77:PRO:HD3	1.93	0.42
1:E:130:LYS:HD3	1:F:78:TRP:HA	2.01	0.42
1:J:163:ARG:HG2	1:J:168:LEU:HD11	2.02	0.42
1:J:242:ASP:N	1:J:242:ASP:OD1	2.52	0.42
1:A:158:GLN:HB3	1:A:161:ARG:HD2	2.01	0.42
1:I:5:ARG:HH12	1:I:62:GLY:H	1.66	0.42
1:G:16:PRO:HB3	1:G:303:LEU:HD13	2.01	0.42
1:A:78:TRP:CG	1:A:128:PRO:HD3	2.54	0.42
1:B:98:TYR:OH	1:B:192:MET:HB3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:TYR:CE1	1:D:300:LEU:HB3	2.55	0.42
1:A:163:ARG:HG2	1:A:168:LEU:HD11	2.01	0.42
1:G:299:TRP:CD1	1:G:300:LEU:HG	2.55	0.41
1:I:27:ILE:HG21	1:I:303:LEU:HD21	2.02	0.41
1:I:78:TRP:CG	1:I:128:PRO:HD3	2.55	0.41
1:C:76:ILE:HA	1:C:77:PRO:HD3	1.92	0.41
1:F:219:ARG:O	1:F:238:TYR:OH	2.32	0.41
1:F:59:VAL:HG11	1:F:285:TYR:CZ	2.55	0.41
1:L:78:TRP:CG	1:L:128:PRO:HD3	2.55	0.41
1:E:229:TYR:OH	1:E:232:GLY:HA2	2.20	0.41
1:L:165:ASN:ND2	1:L:199:PRO:HB2	2.35	0.41
1:L:150:TYR:CD1	1:L:202:LEU:HD22	2.55	0.41
1:E:288:HIS:NE2	1:E:304:LYS:HD2	2.35	0.41
1:D:235:TYR:OH	1:D:314:GLY:O	2.31	0.41
1:D:244:HIS:HB2	1:D:267:PRO:HB3	2.01	0.41
1:B:76:ILE:HB	1:B:79:ALA:HB2	2.02	0.41
1:I:320:LYS:HB2	1:I:320:LYS:HE3	1.86	0.41
1:A:40:ASN:OD1	1:A:41:ASP:N	2.54	0.41
1:K:98:TYR:OH	1:K:192:MET:HB3	2.21	0.41
1:H:85:ASP:O	1:H:137:PRO:HD2	2.20	0.41
1:C:163:ARG:NH2	1:C:172:LEU:O	2.44	0.41
1:K:78:TRP:CG	1:K:128:PRO:HD3	2.56	0.41
1:F:208:LYS:HE2	1:F:208:LYS:HB3	1.91	0.41
1:F:233:LYS:NZ	1:F:235:TYR:OH	2.29	0.41
1:H:245:LEU:HD22	1:H:263:VAL:HG11	2.03	0.41
1:K:227:MET:HB2	1:K:227:MET:HE2	1.94	0.41
1:L:309:LYS:HE2	1:L:309:LYS:HB3	1.87	0.41
1:G:183:PRO:HG2	1:G:202:LEU:HB3	2.03	0.41
1:D:150:TYR:CD1	1:D:202:LEU:HD22	2.56	0.41
1:E:227:MET:HB2	1:E:227:MET:HE2	1.95	0.41
1:A:140:TRP:HA	1:A:141:PRO:HD3	1.93	0.41
1:I:76:ILE:HB	1:I:79:ALA:HB2	2.02	0.40
1:C:113:ALA:HA	1:C:124:PRO:HA	2.03	0.40
1:F:58:ASP:HB3	1:F:62:GLY:HA3	2.04	0.40
1:H:12:TYR:HE1	1:H:294:SER:HB3	1.86	0.40
1:E:180:ALA:HB2	1:E:214:ALA:HA	2.03	0.40
1:B:224:ALA:O	1:B:238:TYR:HA	2.21	0.40
1:I:76:ILE:HA	1:I:77:PRO:HD3	1.93	0.40
1:K:289:HIS:NE2	1:K:301:ARG:HD2	2.36	0.40
1:K:51:TYR:OH	1:K:84:TRP:O	2.25	0.40
1:H:198:GLU:HA	1:H:199:PRO:HD3	1.95	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HG3	1:B:120:GLY:H	1.87	0.40
1:A:222:PHE:HD2	1:A:223:GLU:HG2	1.86	0.40
1:L:163:ARG:HG2	1:L:168:LEU:HD11	2.02	0.40
1:K:37:ILE:HG21	1:K:44:ASP:HB3	2.04	0.40
1:B:163:ARG:HG2	1:B:168:LEU:HD11	2.03	0.40
1:K:87:ASP:OD1	1:K:88:VAL:N	2.52	0.40
1:C:13:MET:HB2	1:C:303:LEU:HG	2.03	0.40
1:I:279:GLU:HB2	1:I:284:TRP:CE2	2.57	0.40
1:B:85:ASP:O	1:B:137:PRO:HD2	2.21	0.40
1:F:15:ASP:H	1:F:289:HIS:HD2	1.68	0.40
1:I:229:TYR:OH	1:I:232:GLY:HA2	2.20	0.40
1:L:198:GLU:HA	1:L:199:PRO:HD3	1.91	0.40
1:B:25:LEU:HD21	1:B:287:PHE:CZ	2.56	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	Percentiles	
1	A	321/324 (99%)	302 (94%)	19 (6%)	0	100	100
1	B	321/324 (99%)	303 (94%)	18 (6%)	0	100	100
1	C	321/324 (99%)	303 (94%)	18 (6%)	0	100	100
1	D	320/324 (99%)	304 (95%)	16 (5%)	0	100	100
1	E	321/324 (99%)	304 (95%)	17 (5%)	0	100	100
1	F	321/324 (99%)	300 (94%)	21 (6%)	0	100	100
1	G	322/324 (99%)	298 (92%)	24 (8%)	0	100	100
1	H	322/324 (99%)	304 (94%)	18 (6%)	0	100	100
1	I	319/324 (98%)	296 (93%)	23 (7%)	0	100	100
1	J	321/324 (99%)	300 (94%)	21 (6%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	322/324 (99%)	302 (94%)	20 (6%)	0	100	100
1	L	320/324 (99%)	301 (94%)	19 (6%)	0	100	100
All	All	3851/3888 (99%)	3617 (94%)	234 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	280/281 (100%)	276 (99%)	4 (1%)	74	92
1	B	280/281 (100%)	275 (98%)	5 (2%)	66	89
1	C	279/281 (99%)	276 (99%)	3 (1%)	80	94
1	D	280/281 (100%)	274 (98%)	6 (2%)	61	87
1	E	280/281 (100%)	278 (99%)	2 (1%)	88	96
1	F	279/281 (99%)	277 (99%)	2 (1%)	88	96
1	G	279/281 (99%)	275 (99%)	4 (1%)	74	92
1	H	280/281 (100%)	277 (99%)	3 (1%)	80	94
1	I	276/281 (98%)	273 (99%)	3 (1%)	80	94
1	J	279/281 (99%)	276 (99%)	3 (1%)	80	94
1	K	280/281 (100%)	273 (98%)	7 (2%)	55	84
1	L	279/281 (99%)	273 (98%)	6 (2%)	60	86
All	All	3351/3372 (99%)	3303 (99%)	48 (1%)	74	92

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	108	PHE
1	A	135	MET
1	A	220	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	108	PHE
1	B	135	MET
1	B	220	ARG
1	B	233	LYS
1	B	297	LYS
1	C	135	MET
1	C	220	ARG
1	C	303	LEU
1	D	11	ASP
1	D	49	LYS
1	D	108	PHE
1	D	135	MET
1	D	220	ARG
1	D	303	LEU
1	E	135	MET
1	E	220	ARG
1	F	135	MET
1	F	220	ARG
1	G	108	PHE
1	G	135	MET
1	G	220	ARG
1	G	266	THR
1	H	135	MET
1	H	200	ARG
1	H	220	ARG
1	I	135	MET
1	I	220	ARG
1	I	231	ASN
1	J	108	PHE
1	J	135	MET
1	J	220	ARG
1	K	108	PHE
1	K	135	MET
1	K	220	ARG
1	K	266	THR
1	K	294	SER
1	K	322	THR
1	K	324	GLU
1	L	135	MET
1	L	220	ARG
1	L	269	VAL
1	L	290	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	301	ARG
1	L	322	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	289	HIS
1	G	45	HIS
1	I	52	HIS
1	K	274	HIS
1	L	165	ASN

### 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](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	402	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	402	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	E	402	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	E	403	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	F	402	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	F	403	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	G	402	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	G	403	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	H	402	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	H	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	I	402	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	I	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	J	402	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	J	403	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	K	402	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	K	403	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	L	402	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	L	403	-	4,4,4	0.23	0	6,6,6	0.07	0

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	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	SO4	B	403	-	-	0/0/0/0	0/0/0/0
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
3	SO4	C	403	-	-	0/0/0/0	0/0/0/0
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	SO4	D	403	-	-	0/0/0/0	0/0/0/0
3	SO4	E	402	-	-	0/0/0/0	0/0/0/0
3	SO4	E	403	-	-	0/0/0/0	0/0/0/0
3	SO4	F	402	-	-	0/0/0/0	0/0/0/0
3	SO4	F	403	-	-	0/0/0/0	0/0/0/0
3	SO4	G	402	-	-	0/0/0/0	0/0/0/0
3	SO4	G	403	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	H	402	-	-	0/0/0/0	0/0/0/0
3	SO4	H	403	-	-	0/0/0/0	0/0/0/0
3	SO4	I	402	-	-	0/0/0/0	0/0/0/0
3	SO4	I	403	-	-	0/0/0/0	0/0/0/0
3	SO4	J	402	-	-	0/0/0/0	0/0/0/0
3	SO4	J	403	-	-	0/0/0/0	0/0/0/0
3	SO4	K	402	-	-	0/0/0/0	0/0/0/0
3	SO4	K	403	-	-	0/0/0/0	0/0/0/0
3	SO4	L	402	-	-	0/0/0/0	0/0/0/0
3	SO4	L	403	-	-	0/0/0/0	0/0/0/0

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

### 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	323/324 (99%)	0.31	15 (4%) 36 35	43, 60, 88, 99	0
1	B	323/324 (99%)	0.42	13 (4%) 42 41	45, 67, 86, 105	0
1	C	323/324 (99%)	0.58	23 (7%) 19 17	50, 78, 112, 146	0
1	D	322/324 (99%)	0.34	7 (2%) 65 66	43, 65, 91, 121	0
1	E	323/324 (99%)	0.41	19 (5%) 26 24	48, 66, 91, 120	0
1	F	323/324 (99%)	0.72	30 (9%) 11 8	49, 75, 104, 131	0
1	G	324/324 (100%)	0.63	19 (5%) 26 24	46, 78, 117, 183	0
1	H	324/324 (100%)	0.61	27 (8%) 14 11	51, 75, 105, 159	0
1	I	321/324 (99%)	0.77	28 (8%) 13 10	53, 76, 109, 148	0
1	J	323/324 (99%)	0.51	17 (5%) 30 28	50, 69, 99, 118	0
1	K	324/324 (100%)	0.74	22 (6%) 20 19	54, 77, 103, 140	0
1	L	322/324 (99%)	1.01	45 (13%) 4 3	58, 89, 123, 151	0
All	All	3875/3888 (99%)	0.59	265 (6%) 20 19	43, 72, 107, 183	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	323	ALA	9.3
1	H	324	GLU	7.3
1	L	42	ASN	5.6
1	G	320	LYS	4.7
1	J	322	THR	4.7
1	F	120	GLY	4.6
1	F	137	PRO	4.5
1	B	136	ASP	4.4
1	H	322	THR	4.4
1	K	177	ASP	4.4
1	B	138	CYS	4.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	138	CYS	4.3
1	I	320	LYS	4.2
1	L	225	SER	4.2
1	G	138	CYS	4.1
1	F	85	ASP	4.0
1	A	136	ASP	4.0
1	I	23	ASP	4.0
1	F	136	ASP	4.0
1	J	175	GLU	3.9
1	G	23	ASP	3.9
1	K	225	SER	3.9
1	I	17	ALA	3.8
1	I	275	HIS	3.7
1	I	86	SER	3.7
1	C	138	CYS	3.7
1	H	214	ALA	3.7
1	K	323	ALA	3.7
1	K	2	LYS	3.6
1	I	322	THR	3.6
1	G	74	GLU	3.6
1	L	210	LYS	3.6
1	L	144	ASP	3.5
1	J	177	ASP	3.5
1	E	36	GLY	3.5
1	L	224	ALA	3.5
1	L	305	VAL	3.4
1	L	85	ASP	3.4
1	J	1	MET	3.4
1	B	225	SER	3.4
1	A	322	THR	3.4
1	I	274	HIS	3.4
1	C	225	SER	3.4
1	G	225	SER	3.3
1	I	136	ASP	3.3
1	C	121	PRO	3.3
1	K	120	GLY	3.2
1	I	39	GLU	3.2
1	H	207	GLU	3.2
1	I	239	SER	3.2
1	I	138	CYS	3.2
1	J	36	GLY	3.2
1	B	137	PRO	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	20	VAL	3.2
1	J	138	CYS	3.1
1	L	137	PRO	3.1
1	F	276	SER	3.1
1	E	37	ILE	3.1
1	F	17	ALA	3.1
1	K	80	GLY	3.1
1	H	225	SER	3.1
1	I	120	GLY	3.1
1	B	86	SER	3.0
1	I	55	SER	3.0
1	G	274	HIS	3.0
1	K	224	ALA	3.0
1	L	276	SER	3.0
1	I	137	PRO	3.0
1	E	41	ASP	3.0
1	L	217	THR	3.0
1	L	121	PRO	3.0
1	L	136	ASP	3.0
1	D	224	ALA	2.9
1	D	23	ASP	2.9
1	E	138	CYS	2.9
1	F	77	PRO	2.9
1	L	172	LEU	2.9
1	B	16	PRO	2.9
1	L	215	GLY	2.9
1	L	274	HIS	2.9
1	F	170	CYS	2.9
1	L	86	SER	2.9
1	F	23	ASP	2.9
1	H	274	HIS	2.8
1	H	94	LYS	2.8
1	C	63	GLU	2.8
1	F	225	SER	2.8
1	H	177	ASP	2.8
1	H	275	HIS	2.8
1	G	85	ASP	2.8
1	H	138	CYS	2.8
1	I	87	ASP	2.8
1	E	10	GLY	2.8
1	J	40	ASN	2.8
1	C	86	SER	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	231	ASN	2.7
1	E	295	LYS	2.7
1	I	85	ASP	2.7
1	H	237	SER	2.7
1	F	2	LYS	2.7
1	L	1	MET	2.7
1	A	62	GLY	2.7
1	H	136	ASP	2.7
1	C	226	TRP	2.7
1	C	275	HIS	2.7
1	D	87	ASP	2.7
1	I	225	SER	2.7
1	C	85	ASP	2.7
1	L	71	LEU	2.7
1	I	224	ALA	2.7
1	H	120	GLY	2.6
1	B	275	HIS	2.6
1	E	61	GLN	2.6
1	D	138	CYS	2.6
1	G	268	VAL	2.6
1	A	224	ALA	2.6
1	H	323	ALA	2.6
1	H	137	PRO	2.6
1	G	120	GLY	2.6
1	H	209	GLY	2.6
1	L	41	ASP	2.6
1	L	242	ASP	2.6
1	H	312	PRO	2.6
1	K	38	PRO	2.6
1	C	322	THR	2.6
1	F	307	GLU	2.6
1	K	87	ASP	2.5
1	F	232	GLY	2.5
1	H	224	ALA	2.5
1	E	177	ASP	2.5
1	K	42	ASN	2.5
1	I	64	VAL	2.5
1	G	299	TRP	2.5
1	B	145	GLY	2.5
1	F	312	PRO	2.5
1	G	53	VAL	2.5
1	K	15	ASP	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	K	138	CYS	2.5
1	F	231	ASN	2.5
1	G	292	VAL	2.5
1	I	63	GLU	2.5
1	A	275	HIS	2.5
1	K	137	PRO	2.5
1	C	291	CYS	2.4
1	L	196	ALA	2.4
1	J	176	GLY	2.4
1	L	176	GLY	2.4
1	E	44	ASP	2.4
1	L	168	LEU	2.4
1	I	15	ASP	2.4
1	A	85	ASP	2.4
1	G	177	ASP	2.4
1	F	286	LEU	2.4
1	H	145	GLY	2.4
1	C	269	VAL	2.4
1	G	318	PRO	2.4
1	J	86	SER	2.4
1	J	225	SER	2.4
1	K	240	THR	2.4
1	F	138	CYS	2.4
1	F	61	GLN	2.4
1	G	137	PRO	2.3
1	K	241	GLY	2.3
1	H	85	ASP	2.3
1	C	2	LYS	2.3
1	L	16	PRO	2.3
1	B	85	ASP	2.3
1	E	224	ALA	2.3
1	C	93	GLY	2.3
1	C	137	PRO	2.3
1	E	86	SER	2.3
1	L	115	SER	2.3
1	L	216	ASP	2.3
1	H	70	VAL	2.3
1	H	211	LEU	2.3
1	A	30	SER	2.3
1	E	225	SER	2.3
1	I	291	CYS	2.3
1	L	19	HIS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	38	PRO	2.3
1	J	41	ASP	2.3
1	K	58	ASP	2.3
1	L	229	TYR	2.3
1	A	63	GLU	2.3
1	E	136	ASP	2.3
1	F	57	ASP	2.3
1	H	213	SER	2.3
1	I	34	GLU	2.3
1	L	313	ASP	2.3
1	L	263	VAL	2.3
1	J	63	GLU	2.2
1	K	23	ASP	2.2
1	L	177	ASP	2.2
1	C	274	HIS	2.2
1	G	323	ALA	2.2
1	F	209	GLY	2.2
1	L	209	GLY	2.2
1	L	40	ASN	2.2
1	C	120	GLY	2.2
1	L	306	ALA	2.2
1	C	268	VAL	2.2
1	I	74	GLU	2.2
1	L	53	VAL	2.2
1	G	136	ASP	2.2
1	L	66	ASP	2.2
1	J	312	PRO	2.2
1	B	226	TRP	2.2
1	A	137	PRO	2.2
1	D	86	SER	2.2
1	F	121	PRO	2.2
1	L	20	VAL	2.2
1	E	85	ASP	2.2
1	F	237	SER	2.2
1	K	176	GLY	2.2
1	G	269	VAL	2.2
1	F	274	HIS	2.2
1	F	266	THR	2.2
1	K	1	MET	2.2
1	L	51	TYR	2.2
1	F	275	HIS	2.2
1	C	224	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	14	ALA	2.2
1	F	224	ALA	2.2
1	F	207	GLU	2.2
1	B	55	SER	2.1
1	L	226	TRP	2.1
1	C	292	VAL	2.1
1	F	226	TRP	2.1
1	C	29	PRO	2.1
1	J	293	PRO	2.1
1	H	230	TYR	2.1
1	L	3	GLU	2.1
1	E	17	ALA	2.1
1	K	45	HIS	2.1
1	J	321	GLY	2.1
1	E	3	GLU	2.1
1	E	207	GLU	2.1
1	F	16	PRO	2.1
1	K	57	ASP	2.1
1	H	232	GLY	2.1
1	A	175	GLU	2.1
1	J	208	LYS	2.1
1	K	320	LYS	2.1
1	B	36	GLY	2.1
1	C	276	SER	2.1
1	I	292	VAL	2.1
1	C	67	HIS	2.1
1	J	85	ASP	2.1
1	I	68	GLY	2.1
1	L	145	GLY	2.1
1	A	134	SER	2.1
1	G	86	SER	2.1
1	H	249	ALA	2.1
1	I	4	PRO	2.0
1	L	318	PRO	2.0
1	E	137	PRO	2.0
1	A	41	ASP	2.0
1	A	116	ASP	2.0
1	E	135	MET	2.0
1	L	291	CYS	2.0
1	A	15	ASP	2.0
1	F	321	GLY	2.0
1	A	2	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	276	SER	2.0
1	D	306	ALA	2.0

## 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(Å <sup>2</sup> )	Q<0.9
3	SO4	I	403	5/5	0.72	0.47	10.34	162,162,163,163	0
3	SO4	K	403	5/5	0.11	0.69	8.16	161,161,161,161	0
2	CA	A	401	1/1	0.91	0.51	5.01	62,62,62,62	0
3	SO4	G	403	5/5	0.53	0.42	4.73	148,149,149,149	0
3	SO4	K	402	5/5	0.75	0.49	4.71	110,110,111,111	0
2	CA	K	401	1/1	0.81	0.53	4.17	81,81,81,81	0
3	SO4	D	403	5/5	0.78	0.29	4.13	113,113,113,114	0
3	SO4	L	403	5/5	0.63	0.52	4.00	152,153,153,153	0
2	CA	B	401	1/1	0.81	0.51	3.95	73,73,73,73	0
2	CA	I	401	1/1	0.96	0.60	3.94	78,78,78,78	0
2	CA	E	401	1/1	0.95	0.47	3.89	70,70,70,70	0
3	SO4	A	402	5/5	0.72	0.59	3.70	109,109,109,109	0
2	CA	C	401	1/1	0.91	0.48	3.67	77,77,77,77	0
3	SO4	G	402	5/5	0.78	0.52	3.47	126,126,126,126	0
2	CA	H	401	1/1	0.86	0.48	3.08	71,71,71,71	0
3	SO4	D	402	5/5	0.90	0.38	2.97	92,93,93,93	0
2	CA	F	401	1/1	0.88	0.54	2.83	84,84,84,84	0
3	SO4	J	403	5/5	0.67	0.47	2.83	153,154,154,154	0
3	SO4	F	403	5/5	0.70	0.28	2.75	136,136,137,137	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	403	5/5	0.72	0.29	2.65	137,137,137,137	0
3	SO4	E	402	5/5	0.83	0.42	2.58	105,105,105,105	0
2	CA	L	401	1/1	0.91	0.50	2.51	80,80,80,80	0
2	CA	J	401	1/1	0.88	0.37	2.36	70,70,70,70	0
3	SO4	H	403	5/5	0.77	0.27	2.33	113,113,114,114	0
3	SO4	F	402	5/5	0.60	0.52	2.31	106,106,107,107	0
2	CA	G	401	1/1	0.84	0.46	2.17	77,77,77,77	0
3	SO4	A	403	5/5	0.73	0.32	1.90	123,123,124,124	0
3	SO4	C	402	5/5	0.78	0.35	1.69	103,103,104,104	0
2	CA	D	401	1/1	0.91	0.36	1.60	65,65,65,65	0
3	SO4	I	402	5/5	0.81	0.42	1.37	105,105,105,106	0
3	SO4	J	402	5/5	0.75	0.33	1.34	101,101,102,102	0
3	SO4	L	402	5/5	0.86	0.36	1.00	111,111,111,111	0
3	SO4	B	402	5/5	0.90	0.35	0.71	85,85,86,86	0
3	SO4	H	402	5/5	0.86	0.31	0.67	94,94,94,95	0
3	SO4	E	403	5/5	0.64	0.26	0.41	131,131,131,131	0
3	SO4	B	403	5/5	0.69	0.18	-0.27	116,116,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.