wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 09:16 PM EDT

PDB ID	:	6WIU
Title	:	Crystal structure of a beta-glucosidase from Exiguobacterium marinum
Authors	:	Zanphorlin, L.M.; Morais, M.A.B.; Murakami, M.T.
Deposited on	:	2020-04-10
Resolution	:	3.51 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*
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:

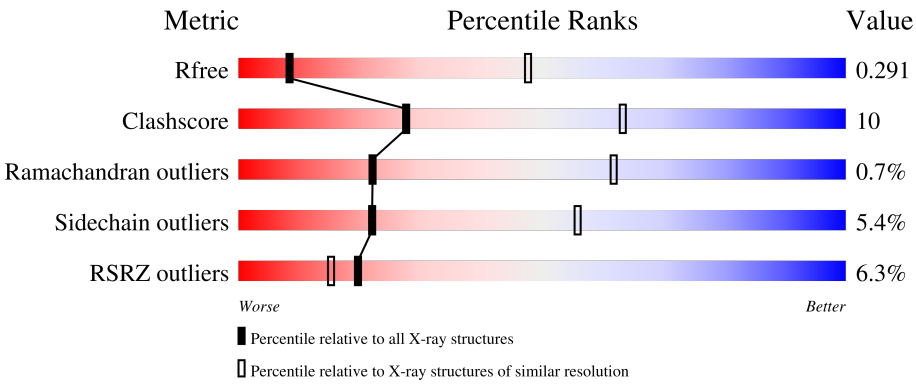
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	471	4% 78% 15% • 6%
1	B	471	4% 73% 19% • 6%
1	C	471	4% 77% 17% 5%
1	D	471	3% 75% 17% • 5%
1	E	471	3% 75% 19% • 5%

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Mol	Chain	Length	Quality of chain
1	F	471	6% 75% 19% 6%
1	G	471	4% 78% 17% 6%
1	H	471	6% 75% 18% 6%
1	I	471	8% 61% 25% 5% 7%
1	J	471	10% 65% 25% 6%
1	K	471	8% 53% 28% 7% 13%
1	L	471	10% 62% 28% 6%
1	M	471	8% 67% 24% 7%
1	N	471	5% 66% 24% 6%
1	O	471	6% 72% 20% 7%
1	P	471	5% 70% 22% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 57949 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-glucosidase.

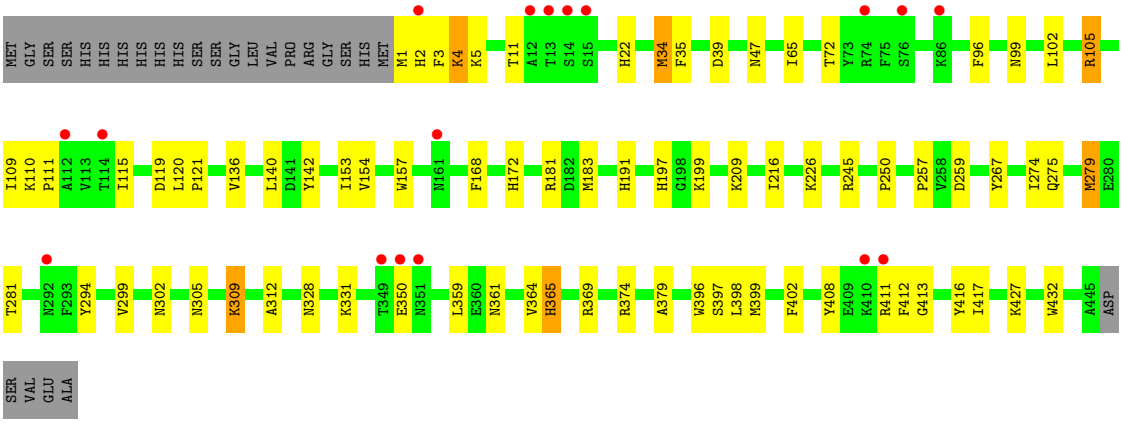
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3653	2337	615	681	20	0	0	0
1	B	444	3648	2334	614	680	20	0	0	0
1	C	446	3661	2342	616	682	21	0	0	0
1	D	446	3661	2342	616	682	21	0	0	0
1	E	447	3669	2346	617	685	21	0	0	0
1	F	445	3653	2337	615	681	20	0	0	0
1	G	444	3648	2334	614	680	20	0	0	0
1	H	445	3653	2337	615	681	20	0	0	0
1	I	438	3600	2304	604	672	20	0	0	0
1	J	444	3648	2334	614	680	20	0	0	0
1	K	412	3375	2160	570	627	18	0	0	0
1	L	443	3638	2328	611	679	20	0	0	0
1	M	438	3597	2301	605	671	20	0	0	0
1	N	441	3618	2313	608	677	20	0	0	0
1	O	438	3588	2293	603	673	19	0	0	0
1	P	443	3639	2329	613	677	20	0	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.

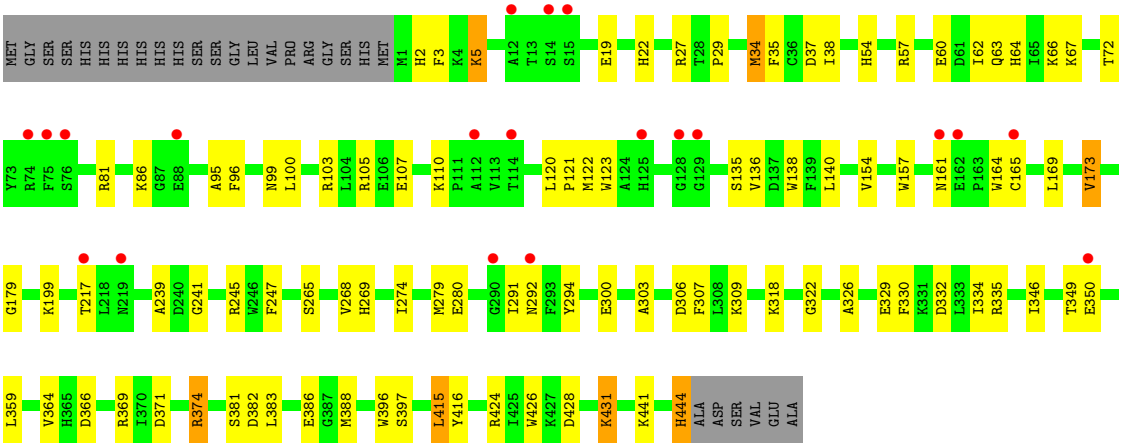
• Molecule 1: Beta-glucosidase

Chain A:



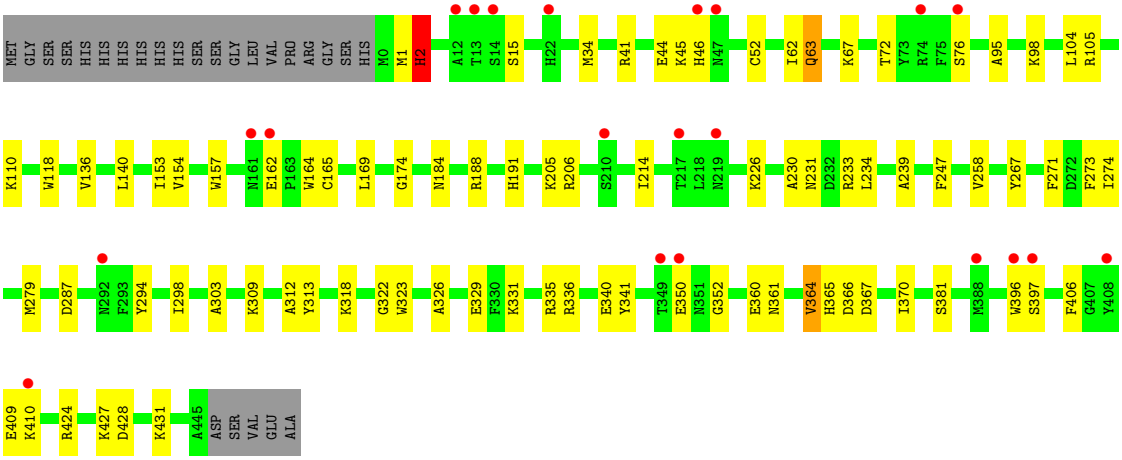
• Molecule 1: Beta-glucosidase

Chain B:



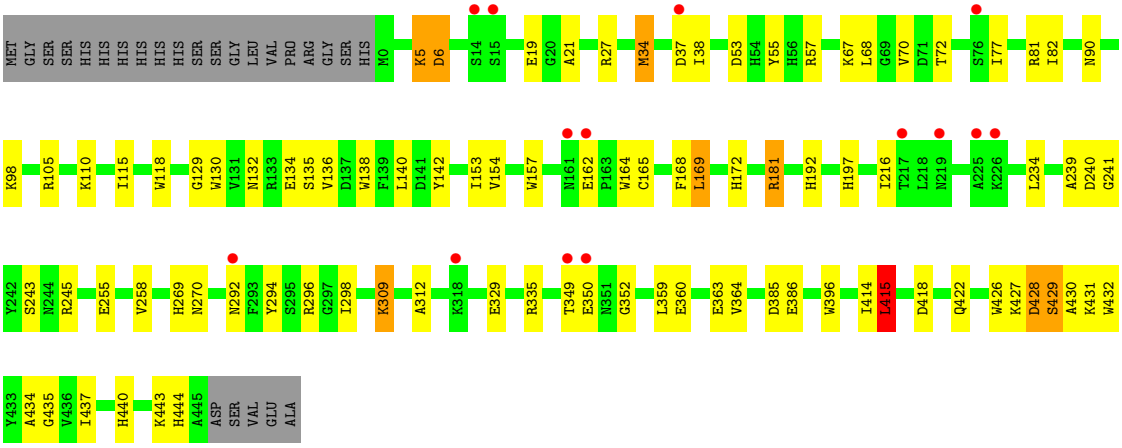
• Molecule 1: Beta-glucosidase

Chain C:



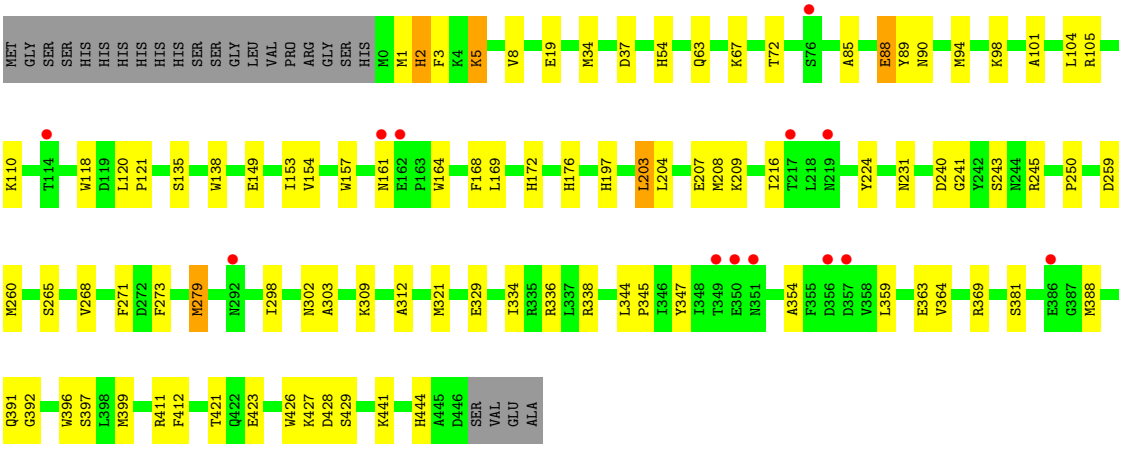
• Molecule 1: Beta-glucosidase

Chain D:



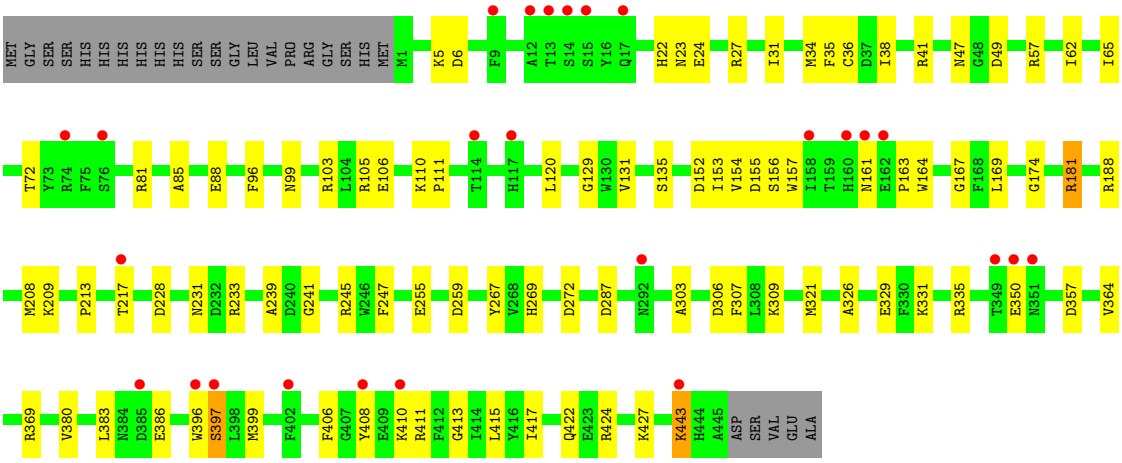
• Molecule 1: Beta-glucosidase

Chain E:



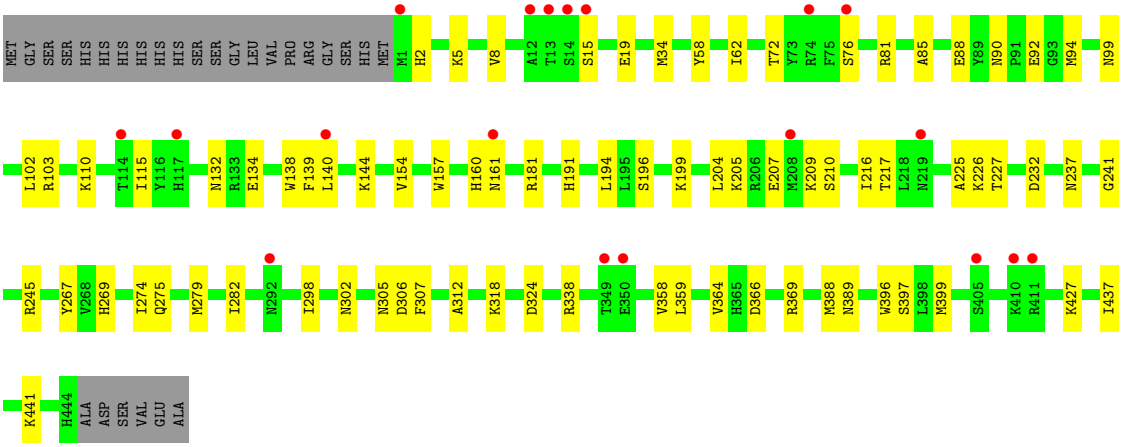
• Molecule 1: Beta-glucosidase

Chain F:



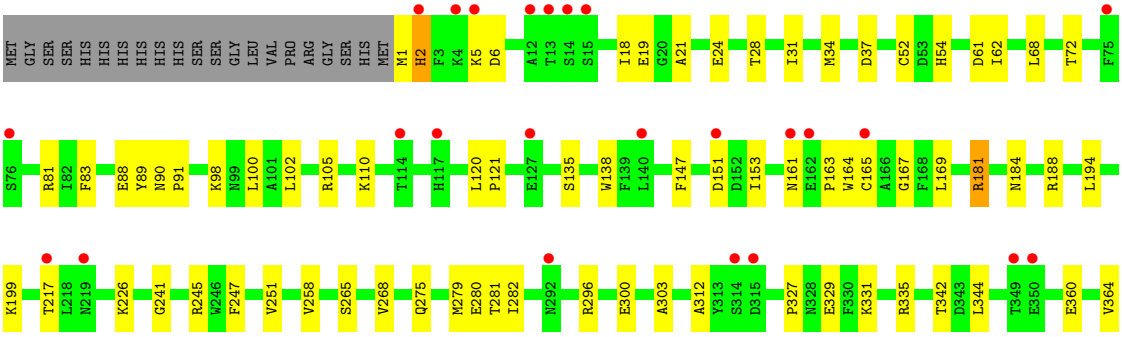
- Molecule 1: Beta-glucosidase

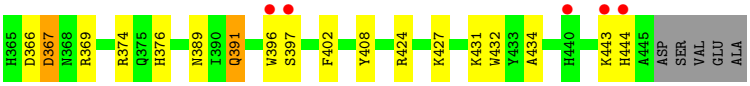
Chain G:



- Molecule 1: Beta-glucosidase

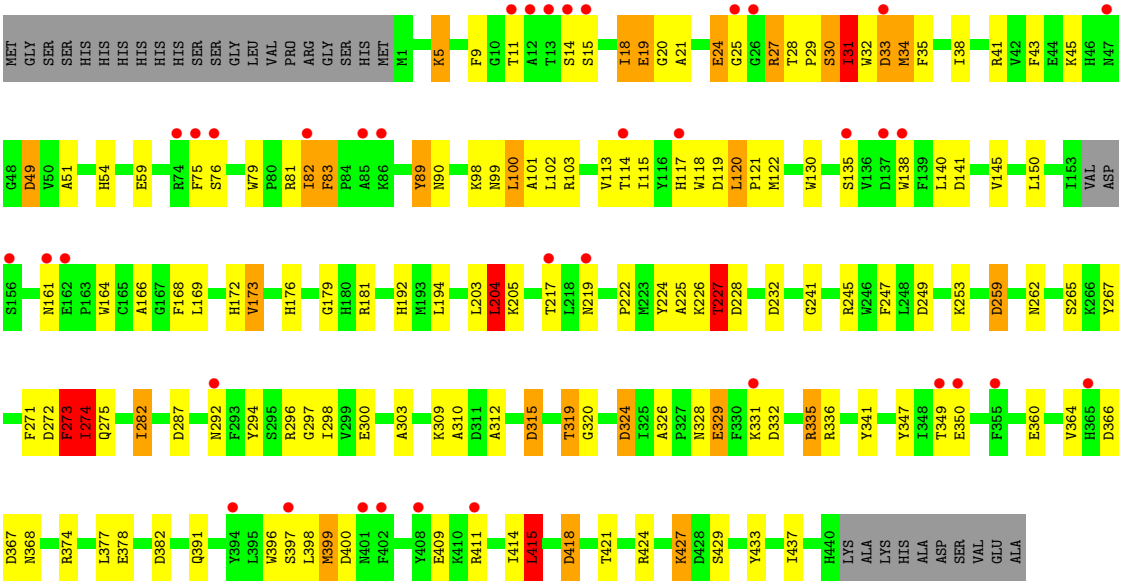
Chain H:





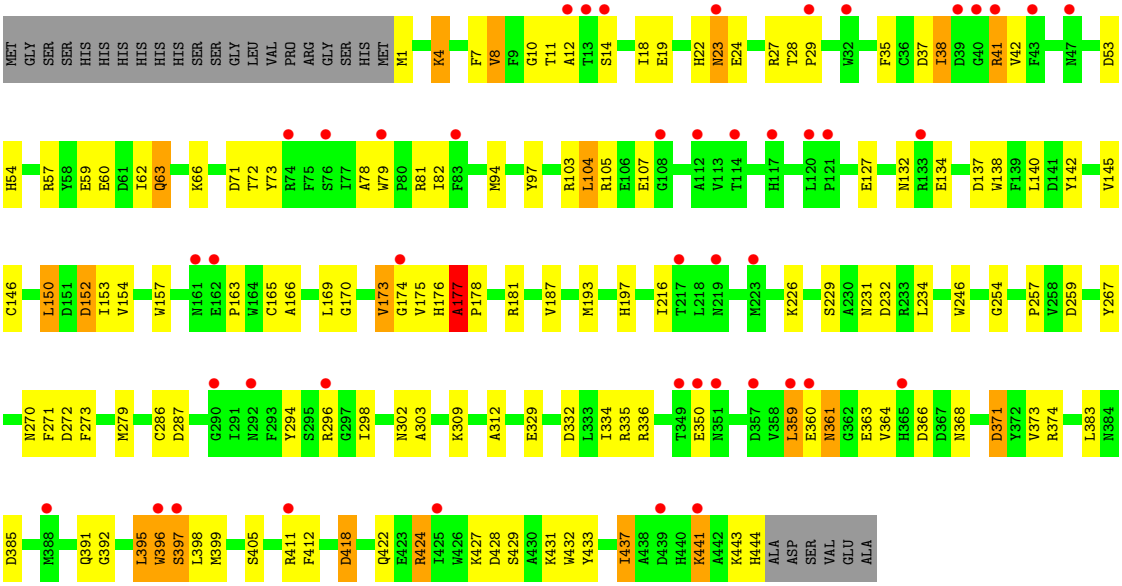
• Molecule 1: Beta-glucosidase

Chain I:



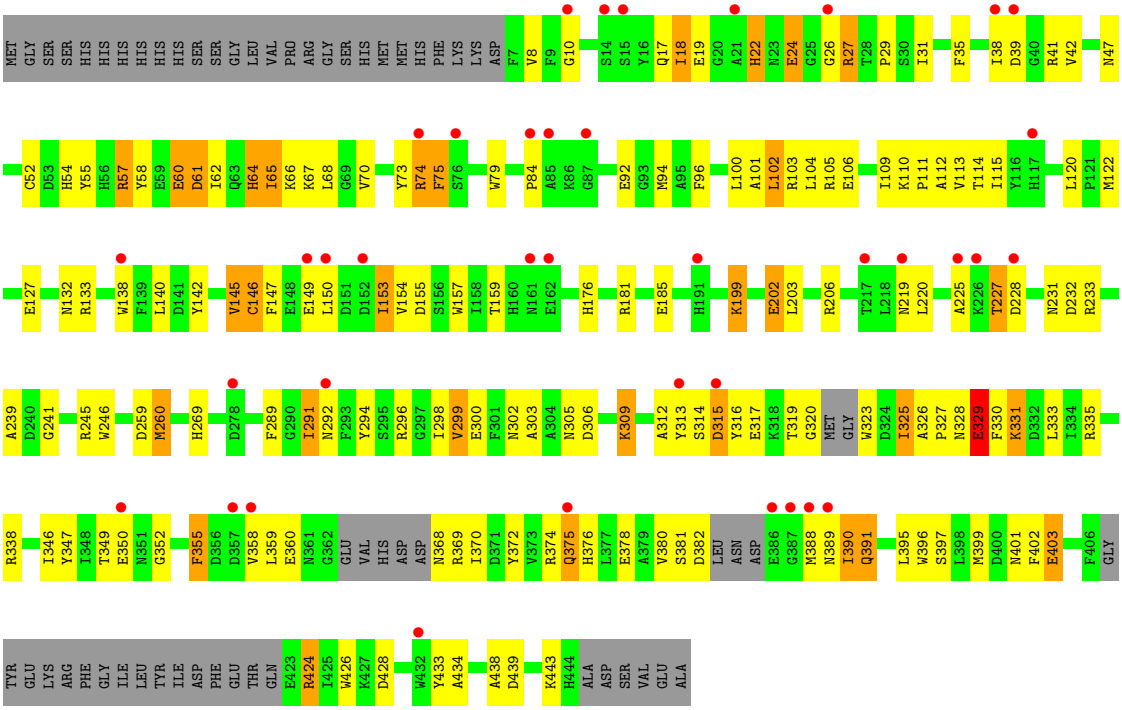
• Molecule 1: Beta-glucosidase

Chain J:



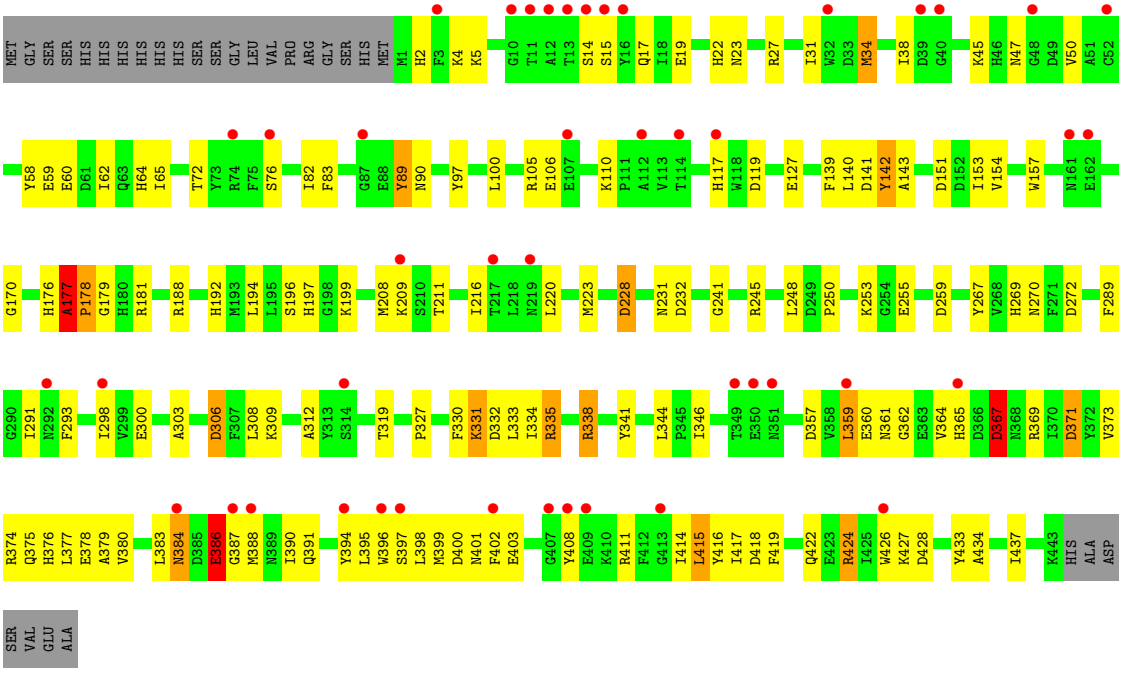
• Molecule 1: Beta-glucosidase

Chain K:



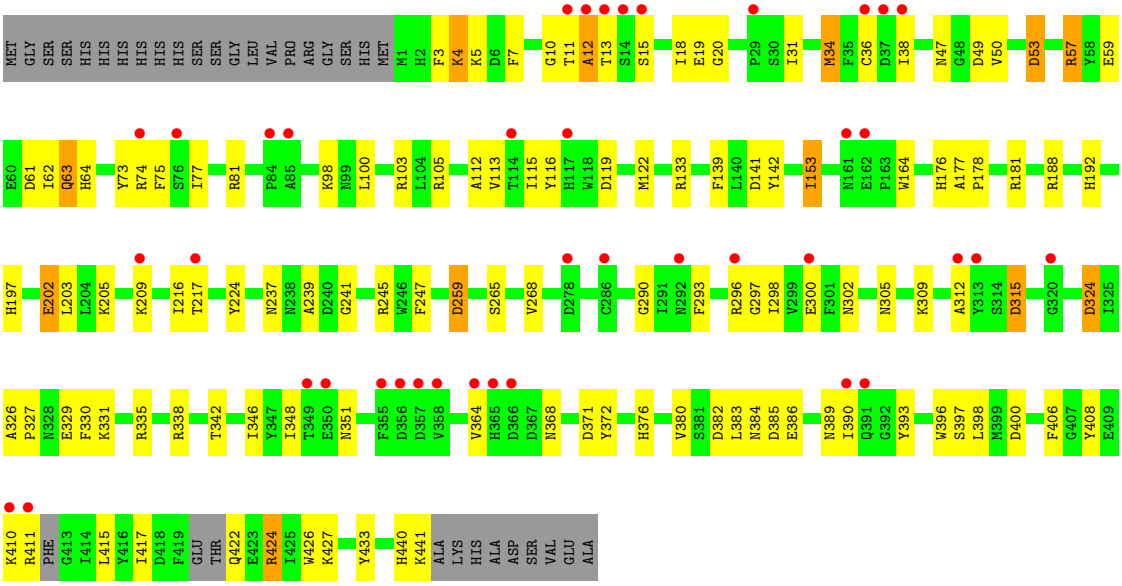
- Molecule 1: Beta-glucosidase

Chain L:



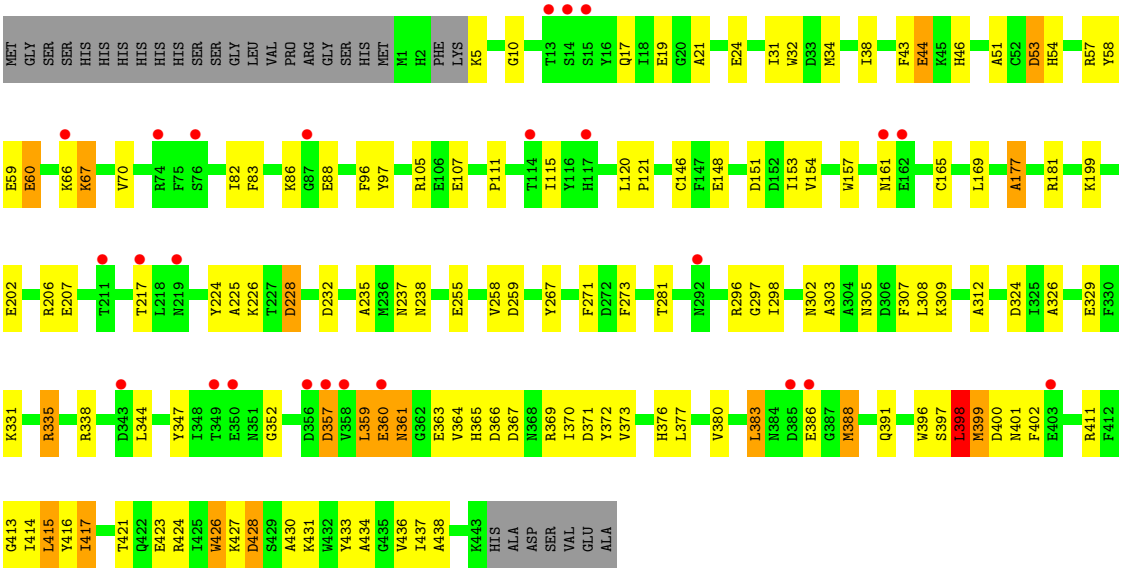
- Molecule 1: Beta-glucosidase

Chain M:



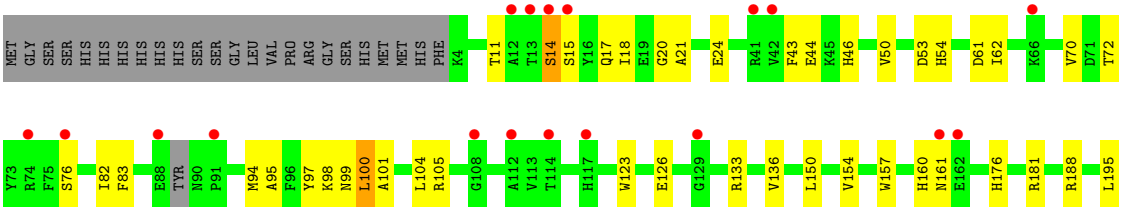
- Molecule 1: Beta-glucosidase

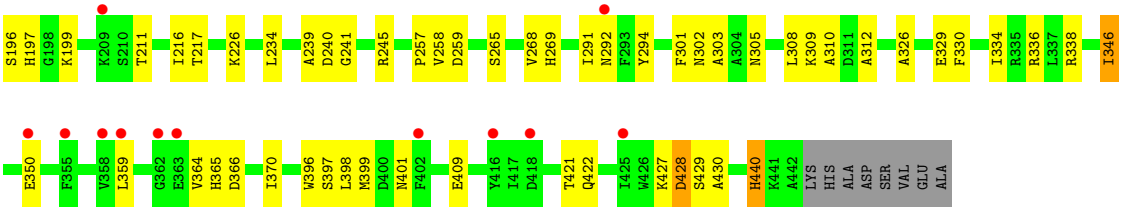
Chain N:



- Molecule 1: Beta-glucosidase

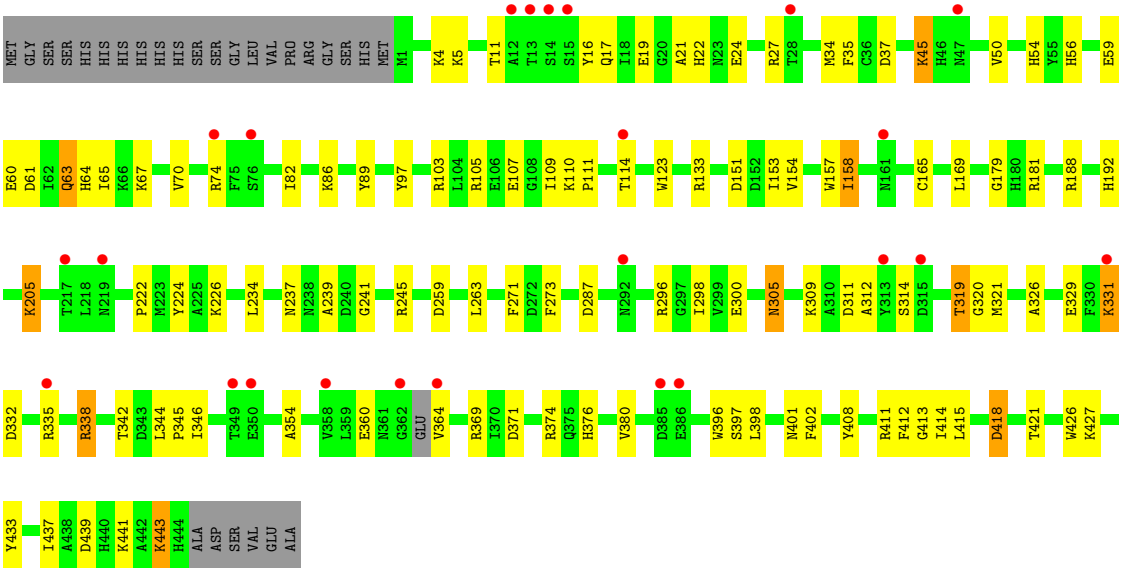
Chain O:





- Molecule 1: Beta-glucosidase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.16Å 171.90Å 213.52Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	32.71 – 3.51 34.15 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.71-3.51) 98.2 (34.15-3.51)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.8.3	Depositor
R, R_{free}	0.263 , 0.292 0.262 , 0.291	Depositor DCC
R_{free} test set	4497 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	94.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 4.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	57949	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.25	0/3765	0.49	0/5102
1	B	0.25	0/3760	0.51	0/5095
1	C	0.25	0/3773	0.50	0/5112
1	D	0.26	0/3773	0.52	2/5112 (0.0%)
1	E	0.24	0/3781	0.48	0/5123
1	F	0.25	0/3765	0.51	0/5102
1	G	0.24	0/3760	0.49	1/5095 (0.0%)
1	H	0.24	0/3765	0.48	0/5102
1	I	0.27	0/3710	0.63	4/5027 (0.1%)
1	J	0.30	0/3760	0.60	1/5095 (0.0%)
1	K	0.30	0/3476	0.70	2/4709 (0.0%)
1	L	0.29	0/3749	0.65	5/5080 (0.1%)
1	M	0.27	0/3705	0.55	2/5018 (0.0%)
1	N	0.28	0/3727	0.61	1/5050 (0.0%)
1	O	0.26	0/3695	0.55	2/5007 (0.0%)
1	P	0.25	0/3750	0.51	1/5080 (0.0%)
All	All	0.26	0/59714	0.55	21/80909 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	L	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	177	ALA	C-N-CD	-9.41	99.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	387	GLY	N-CA-C	-8.10	92.85	113.10
1	L	386	GLU	N-CA-C	7.08	130.13	111.00
1	I	204	LEU	CA-CB-CG	6.85	131.06	115.30
1	I	415	LEU	CA-CB-CG	6.54	130.33	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	240	ASP	Sidechain
1	L	177	ALA	Peptide

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	3653	0	3400	47	0
1	B	3648	0	3395	57	0
1	C	3661	0	3409	58	0
1	D	3661	0	3409	62	0
1	E	3669	0	3413	55	0
1	F	3653	0	3400	64	0
1	G	3648	0	3395	45	0
1	H	3653	0	3400	47	0
1	I	3600	0	3343	100	0
1	J	3648	0	3395	93	2
1	K	3375	0	3138	119	0
1	L	3638	0	3388	109	0
1	M	3597	0	3346	78	2
1	N	3618	0	3365	103	0
1	O	3588	0	3337	57	0
1	P	3639	0	3388	68	0
All	All	57949	0	53921	1115	2

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 10.

The worst 5 of 1115 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:D:364:VAL:HG22	1:D:427:LYS:HD2	1.52	0.92
1:J:66:LYS:HE2	1:J:107:GLU:HG3	1.50	0.90
1:K:241:GLY:HA2	1:K:245:ARG:HG2	1.52	0.90
1:N:105:ARG:NH1	1:N:153:ILE:O	2.05	0.89
1:M:11:THR:HG23	1:M:12:ALA:H	1.37	0.88

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:385:ASP:O	1:M:331:LYS:NZ[2_455]	2.16	0.04
1:J:385:ASP:OD2	1:M:335:ARG:NH2[2_455]	2.19	0.01

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	443/471 (94%)	426 (96%)	16 (4%)	1 (0%)	47	80
1	B	442/471 (94%)	427 (97%)	14 (3%)	1 (0%)	47	80
1	C	444/471 (94%)	427 (96%)	16 (4%)	1 (0%)	47	80
1	D	444/471 (94%)	424 (96%)	17 (4%)	3 (1%)	22	62
1	E	445/471 (94%)	426 (96%)	18 (4%)	1 (0%)	47	80
1	F	443/471 (94%)	423 (96%)	19 (4%)	1 (0%)	47	80
1	G	442/471 (94%)	424 (96%)	18 (4%)	0	100	100
1	H	443/471 (94%)	426 (96%)	16 (4%)	1 (0%)	47	80
1	I	434/471 (92%)	400 (92%)	22 (5%)	12 (3%)	5	34
1	J	442/471 (94%)	412 (93%)	25 (6%)	5 (1%)	14	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	402/471 (85%)	360 (90%)	29 (7%)	13 (3%)	4	31
1	L	441/471 (94%)	413 (94%)	22 (5%)	6 (1%)	11	47
1	M	432/471 (92%)	414 (96%)	18 (4%)	0	100	100
1	N	437/471 (93%)	416 (95%)	20 (5%)	1 (0%)	47	80
1	O	434/471 (92%)	411 (95%)	19 (4%)	4 (1%)	17	57
1	P	439/471 (93%)	418 (95%)	19 (4%)	2 (0%)	29	67
All	All	7007/7536 (93%)	6647 (95%)	308 (4%)	52 (1%)	22	62

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	429	SER
1	E	428	ASP
1	I	30	SER
1	I	31	ILE
1	I	49	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/401 (94%)	365 (96%)	14 (4%)	34	65
1	B	379/401 (94%)	369 (97%)	10 (3%)	46	74
1	C	380/401 (95%)	375 (99%)	5 (1%)	69	86
1	D	380/401 (95%)	370 (97%)	10 (3%)	46	74
1	E	381/401 (95%)	370 (97%)	11 (3%)	42	71
1	F	379/401 (94%)	372 (98%)	7 (2%)	59	81
1	G	379/401 (94%)	370 (98%)	9 (2%)	49	76
1	H	379/401 (94%)	364 (96%)	15 (4%)	31	64
1	I	374/401 (93%)	335 (90%)	39 (10%)	7	32
1	J	379/401 (94%)	344 (91%)	35 (9%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	350/401 (87%)	303 (87%)	47 (13%)	4	22
1	L	378/401 (94%)	345 (91%)	33 (9%)	10	39
1	M	374/401 (93%)	350 (94%)	24 (6%)	17	51
1	N	376/401 (94%)	346 (92%)	30 (8%)	12	42
1	O	373/401 (93%)	358 (96%)	15 (4%)	31	64
1	P	378/401 (94%)	355 (94%)	23 (6%)	18	52
All	All	6018/6416 (94%)	5691 (95%)	327 (5%)	22	56

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	415	LEU
1	N	426	TRP
1	M	34	MET
1	N	44	GLU
1	O	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	351	ASN
1	L	270	ASN
1	P	231	ASN
1	O	270	ASN
1	P	17	GLN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 95th 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^2)	Q<0.9
1	A	445/471 (94%)	-0.09	17 (3%)	40	30	64, 78, 100, 196	0
1	B	444/471 (94%)	0.07	20 (4%)	33	24	65, 96, 125, 197	0
1	C	446/471 (94%)	-0.01	21 (4%)	31	23	66, 82, 99, 185	0
1	D	446/471 (94%)	0.04	14 (3%)	49	36	64, 88, 111, 166	0
1	E	447/471 (94%)	-0.17	13 (2%)	51	38	63, 82, 106, 147	0
1	F	445/471 (94%)	0.14	26 (5%)	23	17	65, 97, 124, 281	0
1	G	444/471 (94%)	-0.02	19 (4%)	35	26	63, 91, 115, 215	0
1	H	445/471 (94%)	0.13	29 (6%)	18	14	64, 90, 115, 159	0
1	I	438/471 (92%)	0.35	37 (8%)	11	9	80, 118, 170, 267	0
1	J	444/471 (94%)	0.36	45 (10%)	7	6	77, 111, 152, 460	0
1	K	412/471 (87%)	0.35	38 (9%)	9	7	90, 139, 204, 347	0
1	L	443/471 (94%)	0.34	45 (10%)	6	6	83, 111, 151, 205	0
1	M	438/471 (92%)	0.36	40 (9%)	9	7	76, 112, 143, 245	0
1	N	441/471 (93%)	0.12	25 (5%)	23	17	77, 106, 149, 430	0
1	O	438/471 (92%)	0.26	30 (6%)	17	14	81, 106, 154, 276	0
1	P	443/471 (94%)	0.12	24 (5%)	25	19	75, 98, 124, 185	0
All	All	7059/7536 (93%)	0.14	443 (6%)	20	15	63, 98, 149, 460	0

The worst 5 of 443 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	161	ASN	6.8
1	K	386	GLU	6.6
1	K	292	ASN	6.3
1	I	292	ASN	6.1
1	L	76	SER	5.7

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.