wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:21 PM GMT

PDB ID	:	4V44
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH 2-F-LACTOSE
Authors	:	Juers, D.H.; McCarter, J.D.; Withers, S.G.; Matthews, B.W.
Deposited on	:	2001-09-13
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

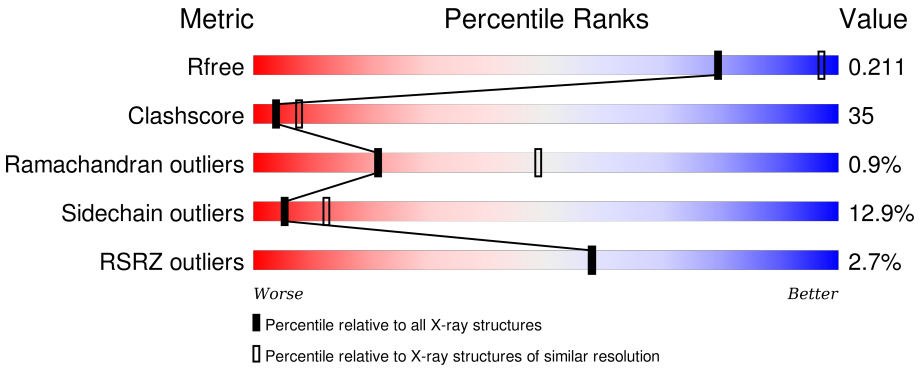
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 >=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 <=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	1023	% 43% 42% 13% •
1	B	1023	% 43% 42% 13% •
1	C	1023	% 44% 41% 12% •
1	D	1023	% 43% 42% 13% •
1	E	1023	4% 43% 42% 13% •

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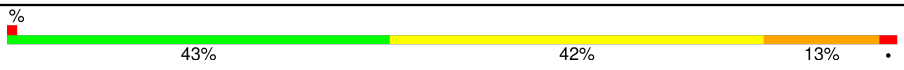
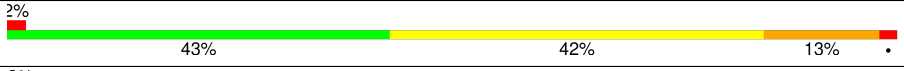
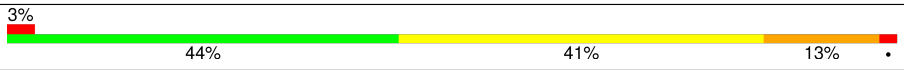
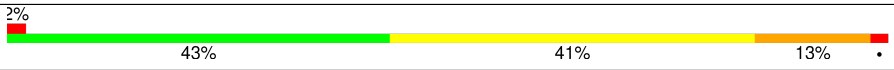
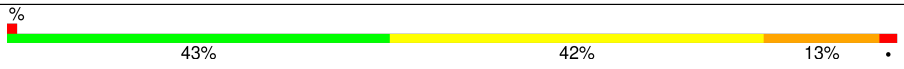
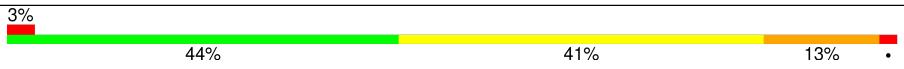
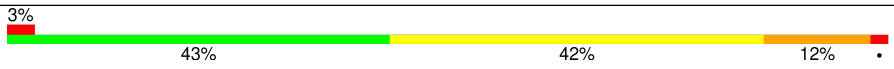
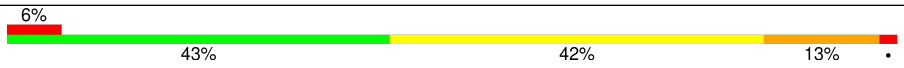
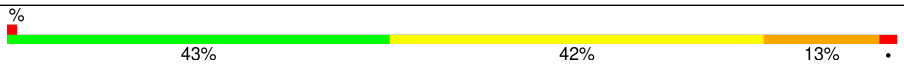
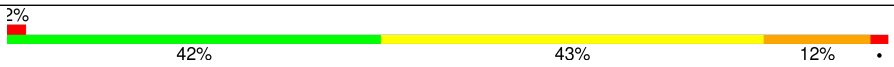
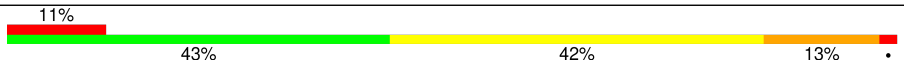
Mol	Chain	Length	Quality of chain
1	F	1023	
1	G	1023	
1	H	1023	
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	

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
1	CME	A	1021	-	-	X	-
1	CME	B	1021	-	-	X	-
1	CME	C	1021	-	-	X	-
1	CME	D	1021	-	-	X	-
1	CME	E	1021	-	-	X	-
1	CME	F	1021	-	-	X	-
1	CME	G	1021	-	-	X	-
1	CME	H	1021	-	-	X	-
1	CME	I	1021	-	-	X	-
1	CME	J	1021	-	-	X	-
1	CME	K	1021	-	-	X	-
1	CME	L	1021	-	-	X	-
1	CME	M	1021	-	-	X	-
1	CME	N	1021	-	-	X	-
1	CME	O	1021	-	-	X	-
1	CME	P	1021	-	-	X	-
2	2FL	B	2001	-	-	-	X
2	2FL	C	2001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FL	D	2001	-	-	-	X
2	2FL	E	2001	-	-	-	X
2	2FL	F	2001	-	-	-	X
2	2FL	G	2001	-	-	-	X
2	2FL	H	2001	-	-	-	X
2	2FL	J	2001	-	-	-	X
2	2FL	K	2001	-	-	-	X
2	2FL	L	2001	-	-	-	X
2	2FL	O	2001	-	-	-	X
3	MG	B	2002	-	-	-	X
3	MG	C	2002	-	-	-	X
3	MG	D	2002	-	-	-	X
3	MG	F	2002	-	-	-	X
3	MG	G	2002	-	-	-	X
3	MG	H	2002	-	-	-	X
3	MG	I	2002	-	-	-	X
3	MG	N	2002	-	-	-	X
3	MG	O	2002	-	-	-	X
4	NA	B	2005	-	-	-	X
4	NA	E	2004	-	-	-	X
4	NA	F	2005	-	-	-	X
4	NA	J	2004	-	-	-	X
4	NA	J	2005	-	-	-	X
4	NA	K	2004	-	-	-	X
4	NA	L	2004	-	-	-	X
4	NA	M	2004	-	-	-	X
4	NA	N	2005	-	-	-	X
4	NA	O	2005	-	-	-	X
4	NA	P	2004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 134528 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-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	B	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	C	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	D	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	E	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	F	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	G	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	H	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	I	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	J	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	K	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	L	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	M	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	N	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	O	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	P	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
A	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
A	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
B	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
B	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
B	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
C	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
C	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
C	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
D	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
D	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
D	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
E	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
E	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
E	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
F	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
F	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
F	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
G	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
G	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
G	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
H	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
H	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
H	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
I	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
I	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
I	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
M	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
M	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
M	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722

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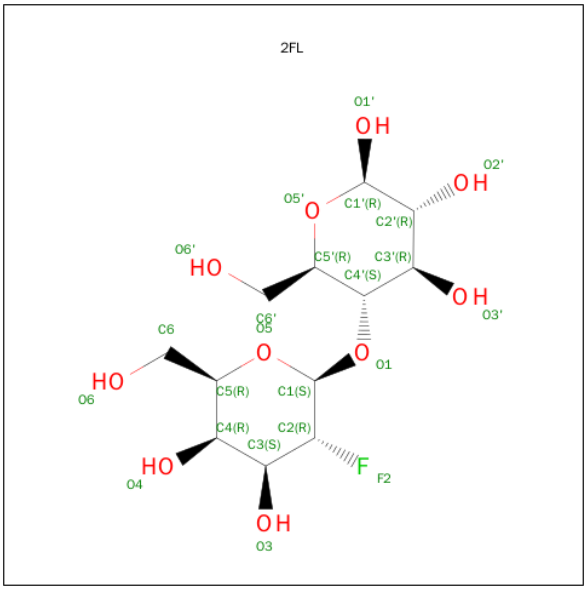
Chain	Residue	Modelled	Actual	Comment	Reference
O	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
O	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
O	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722

- Molecule 2 is SUGAR (2-FLUORO-2-DEOXY-LACTOSE) (three-letter code: 2FL) (formula: $C_{12}H_{21}FO_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			23	12	1	10		
2	B	1	Total	C	F	O	0	0
			23	12	1	10		
2	C	1	Total	C	F	O	0	0
			23	12	1	10		
2	D	1	Total	C	F	O	0	0
			23	12	1	10		
2	E	1	Total	C	F	O	0	0
			23	12	1	10		
2	F	1	Total	C	F	O	0	0
			23	12	1	10		
2	G	1	Total	C	F	O	0	0
			23	12	1	10		
2	H	1	Total	C	F	O	0	0
			23	12	1	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C F O 23 12 1 10	0	0
2	J	1	Total C F O 23 12 1 10	0	0
2	K	1	Total C F O 23 12 1 10	0	0
2	L	1	Total C F O 23 12 1 10	0	0
2	M	1	Total C F O 23 12 1 10	0	0
2	N	1	Total C F O 23 12 1 10	0	0
2	O	1	Total C F O 23 12 1 10	0	0
2	P	1	Total C F O 23 12 1 10	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	K	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	I	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	2	Total Mg 2 2	0	0
3	O	2	Total Mg 2 2	0	0
3	L	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0
3	M	2	Total Mg 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	2	Total Na 2 2	0	0
4	G	2	Total Na 2 2	0	0
4	J	2	Total Na 2 2	0	0
4	D	2	Total Na 2 2	0	0
4	K	2	Total Na 2 2	0	0
4	E	2	Total Na 2 2	0	0
4	H	2	Total Na 2 2	0	0
4	B	2	Total Na 2 2	0	0
4	I	2	Total Na 2 2	0	0
4	C	2	Total Na 2 2	0	0
4	A	2	Total Na 2 2	0	0
4	N	2	Total Na 2 2	0	0
4	O	2	Total Na 2 2	0	0
4	L	2	Total Na 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total Na 2 2	0	0
4	M	2	Total Na 2 2	0	0

- Molecule 5 is water.

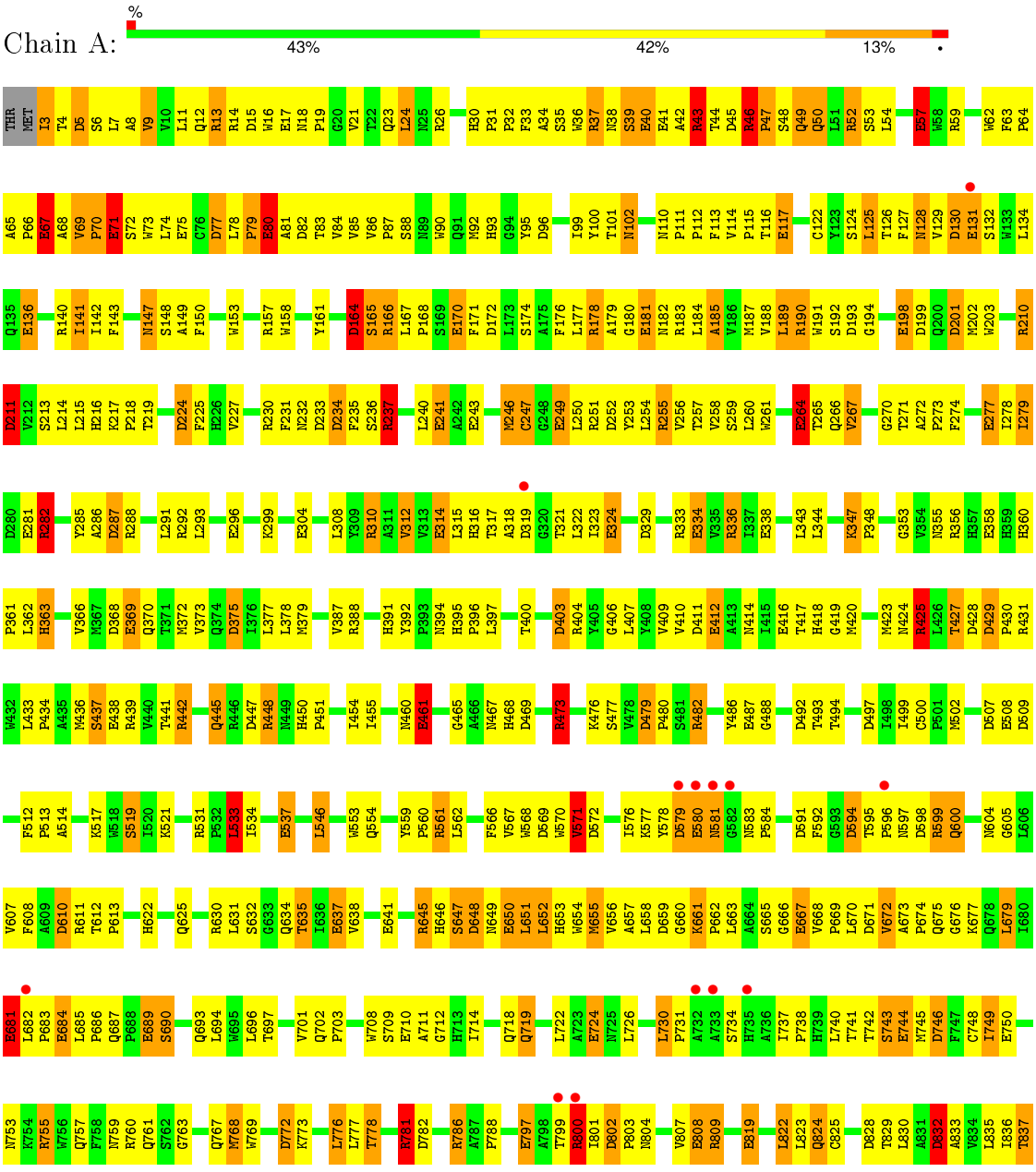
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	160	Total O 160 160	0	0
5	B	163	Total O 163 163	0	0
5	C	162	Total O 162 162	0	0
5	D	163	Total O 163 163	0	0
5	E	162	Total O 162 162	0	0
5	F	162	Total O 162 162	0	0
5	G	162	Total O 162 162	0	0
5	H	162	Total O 162 162	0	0
5	I	162	Total O 162 162	0	0
5	J	162	Total O 162 162	0	0
5	K	162	Total O 162 162	0	0
5	L	162	Total O 162 162	0	0
5	M	161	Total O 161 161	0	0
5	N	163	Total O 163 163	0	0
5	O	161	Total O 161 161	0	0
5	P	163	Total O 163 163	0	0

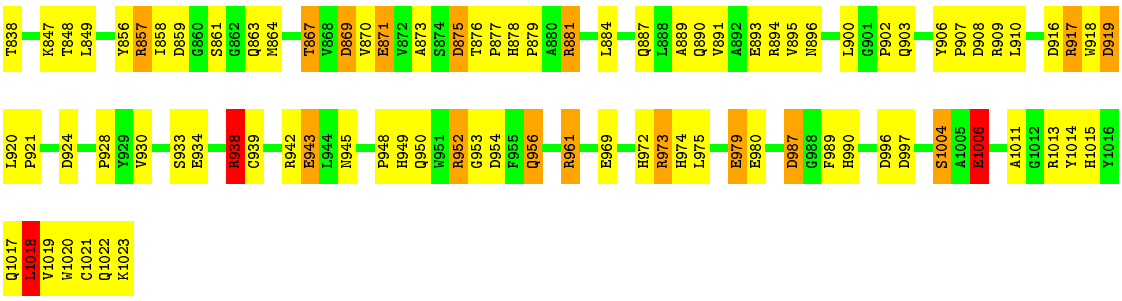
3 Residue-property plots (i)

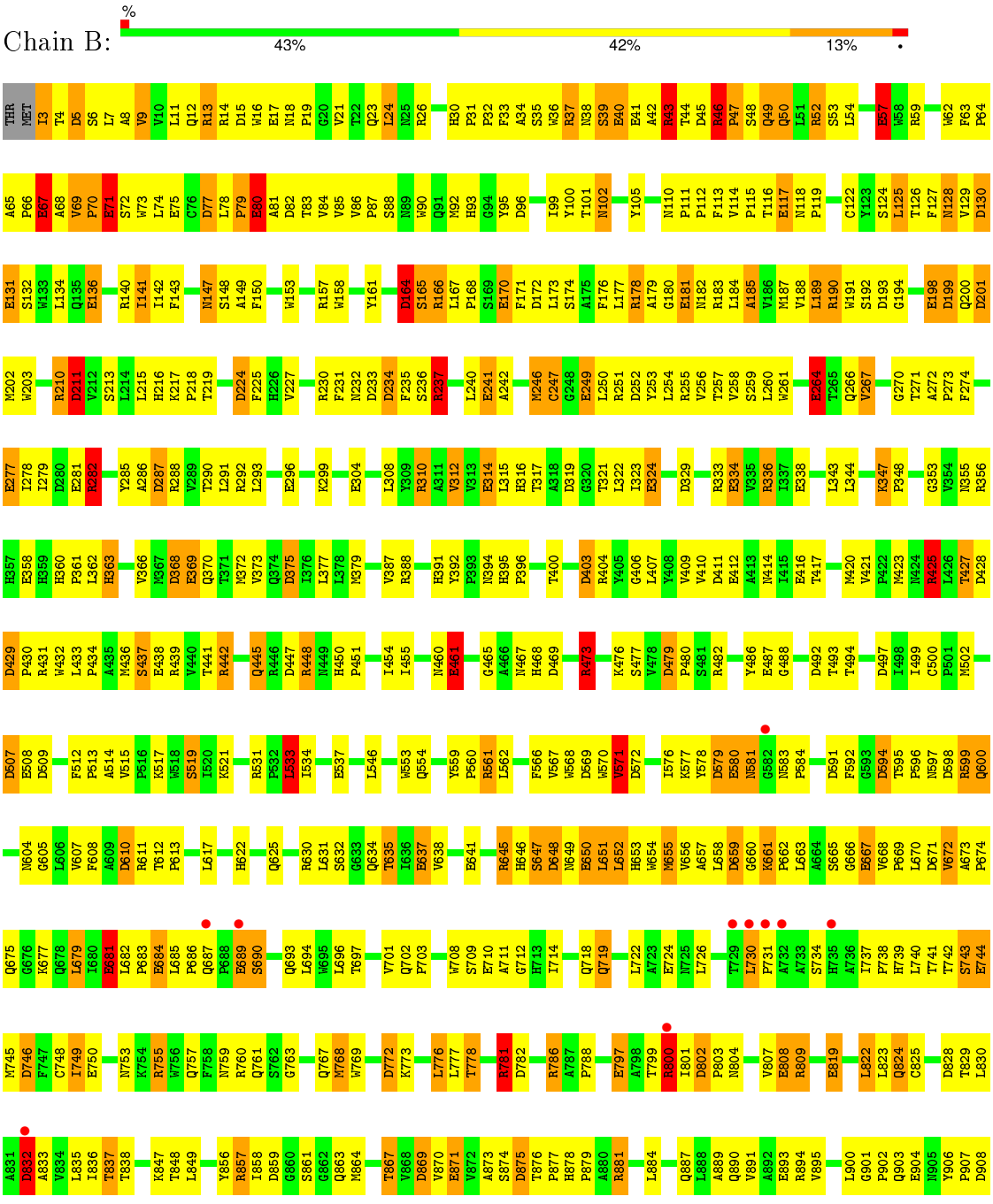
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain A:

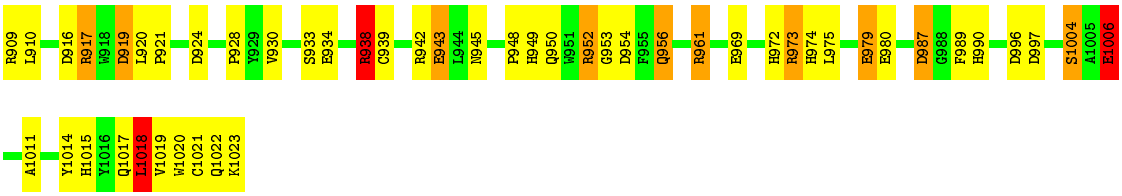


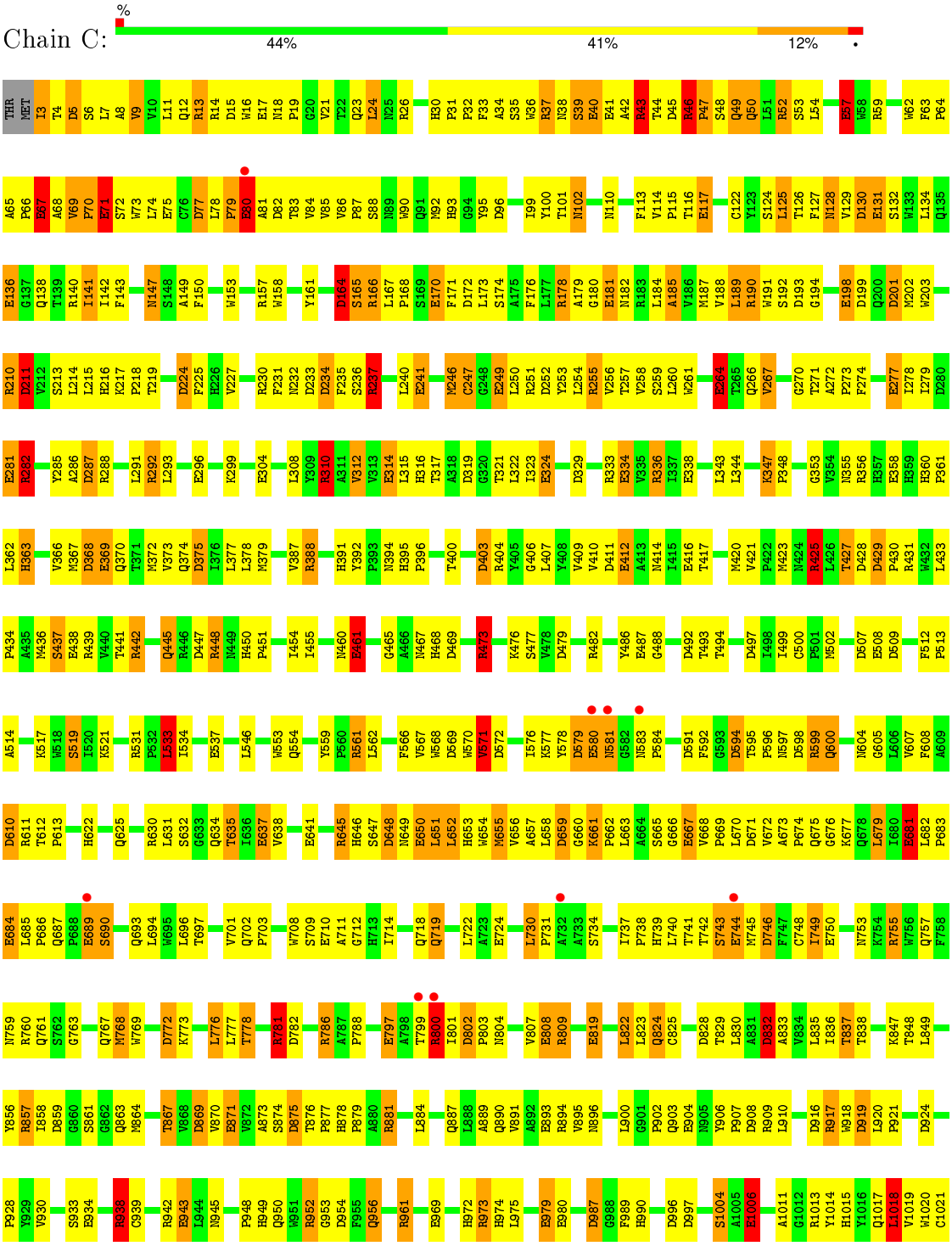




• Molecule 1: Beta-Galactosidase

Chain B:



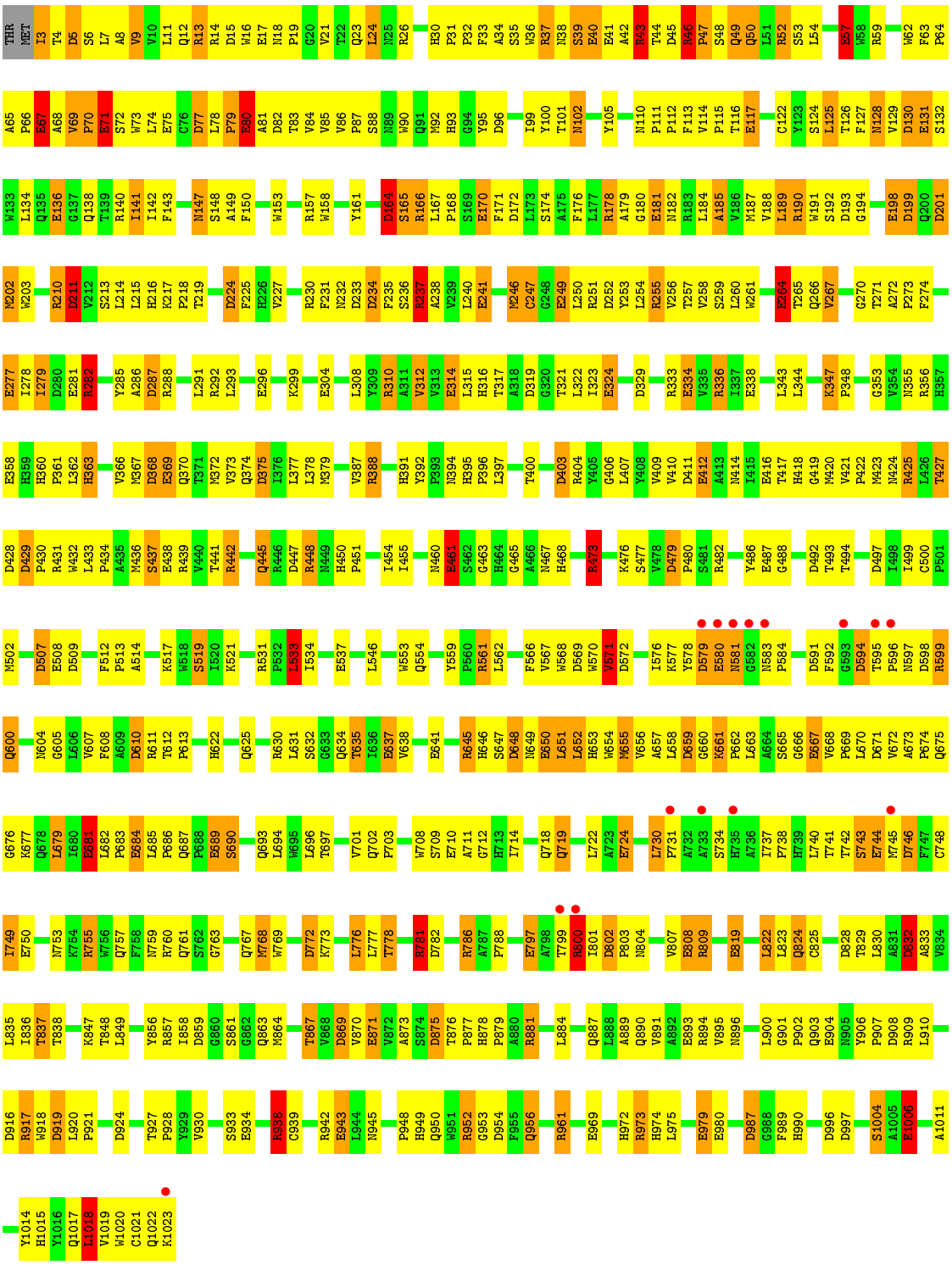


• Molecule 1: Beta-Galactosidase

Chain C:

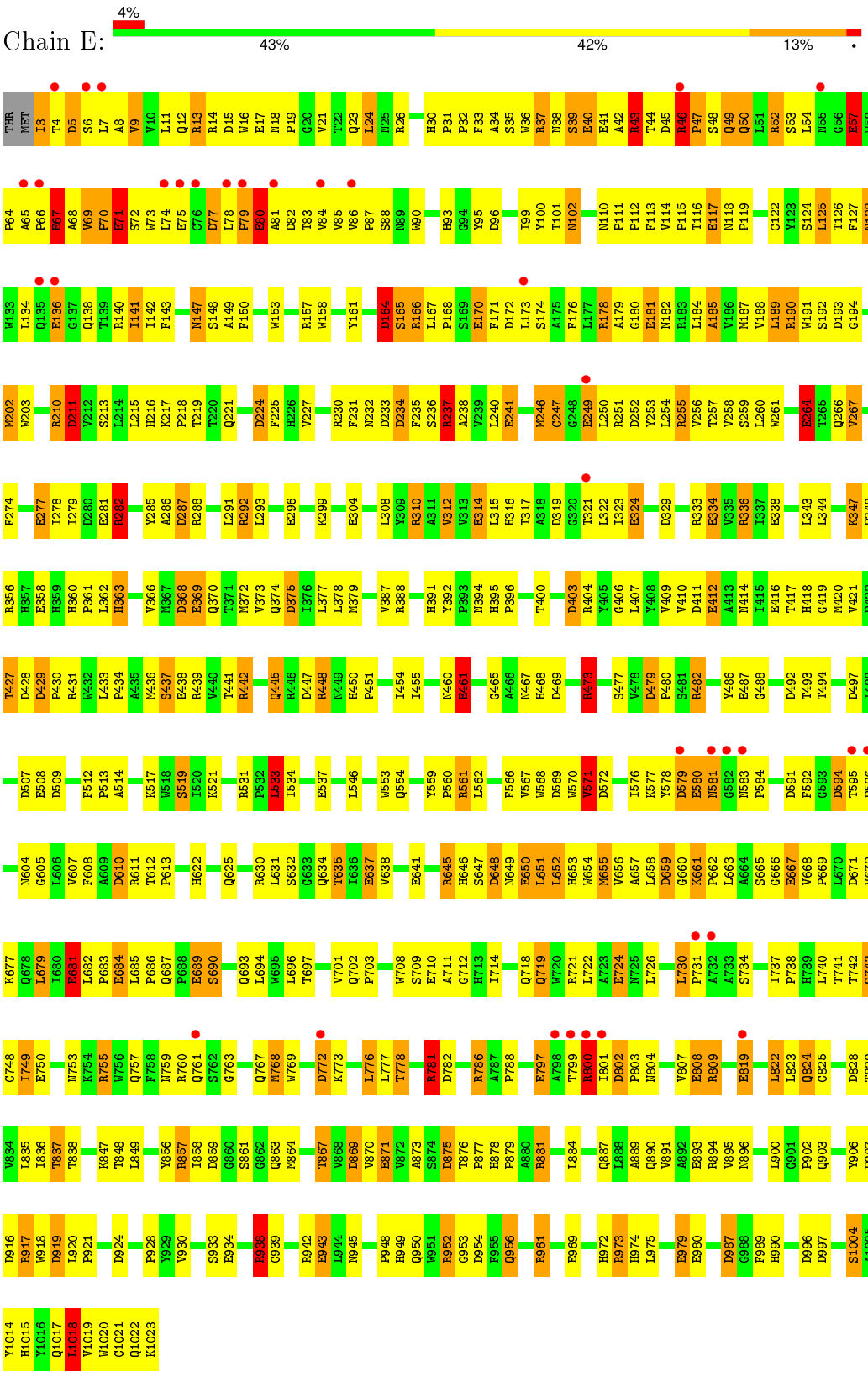
• Molecule 1: Beta-Galactosidase

Chain D:



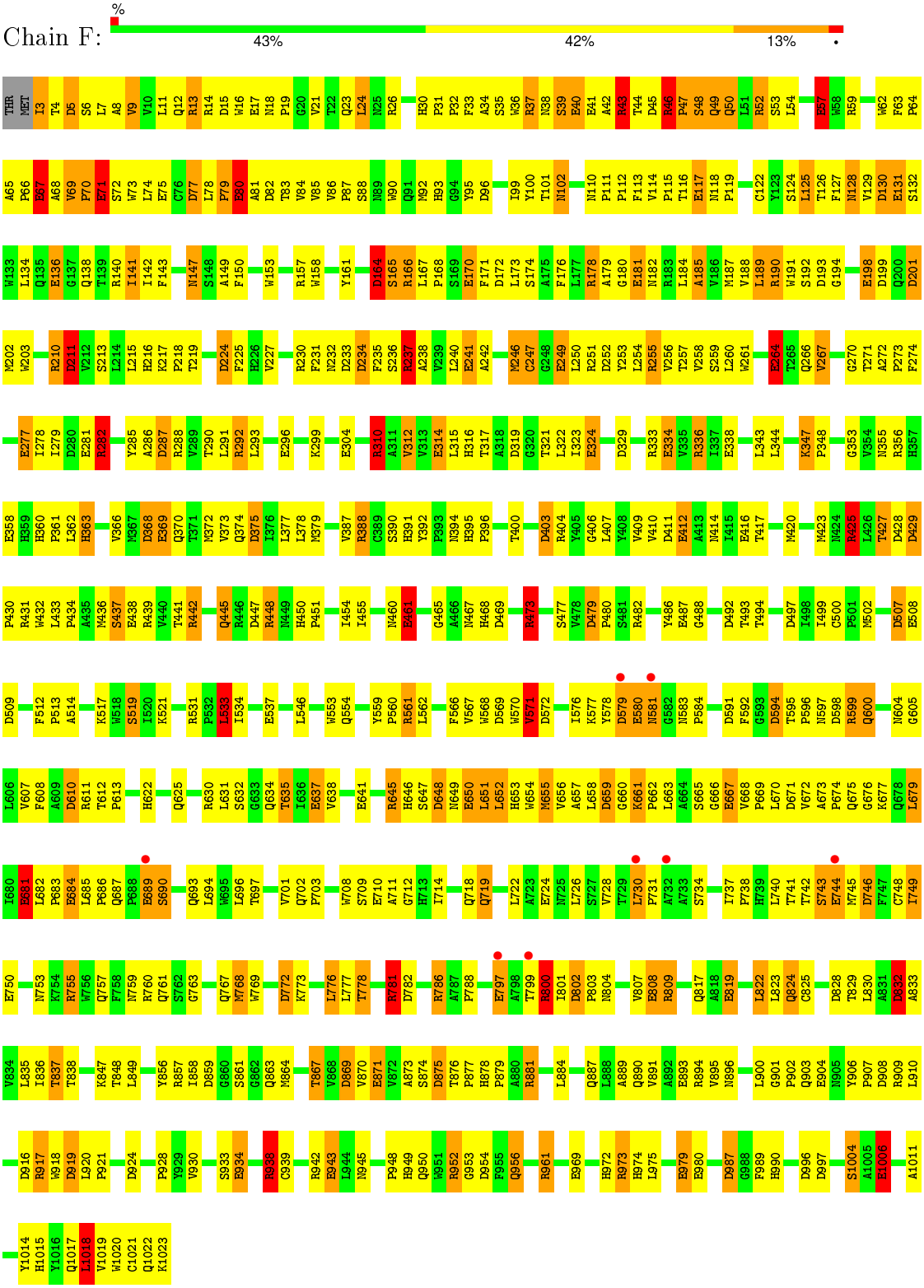
• Molecule 1: Beta-Galactosidase

Chain E:



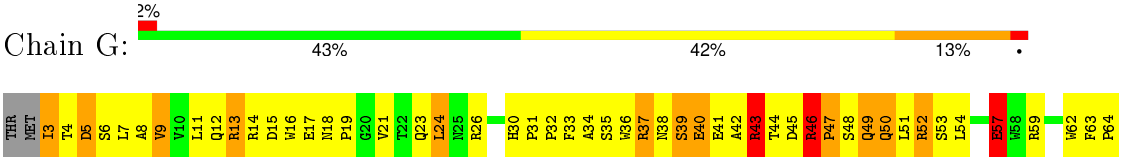
• Molecule 1: Beta-Galactosidase

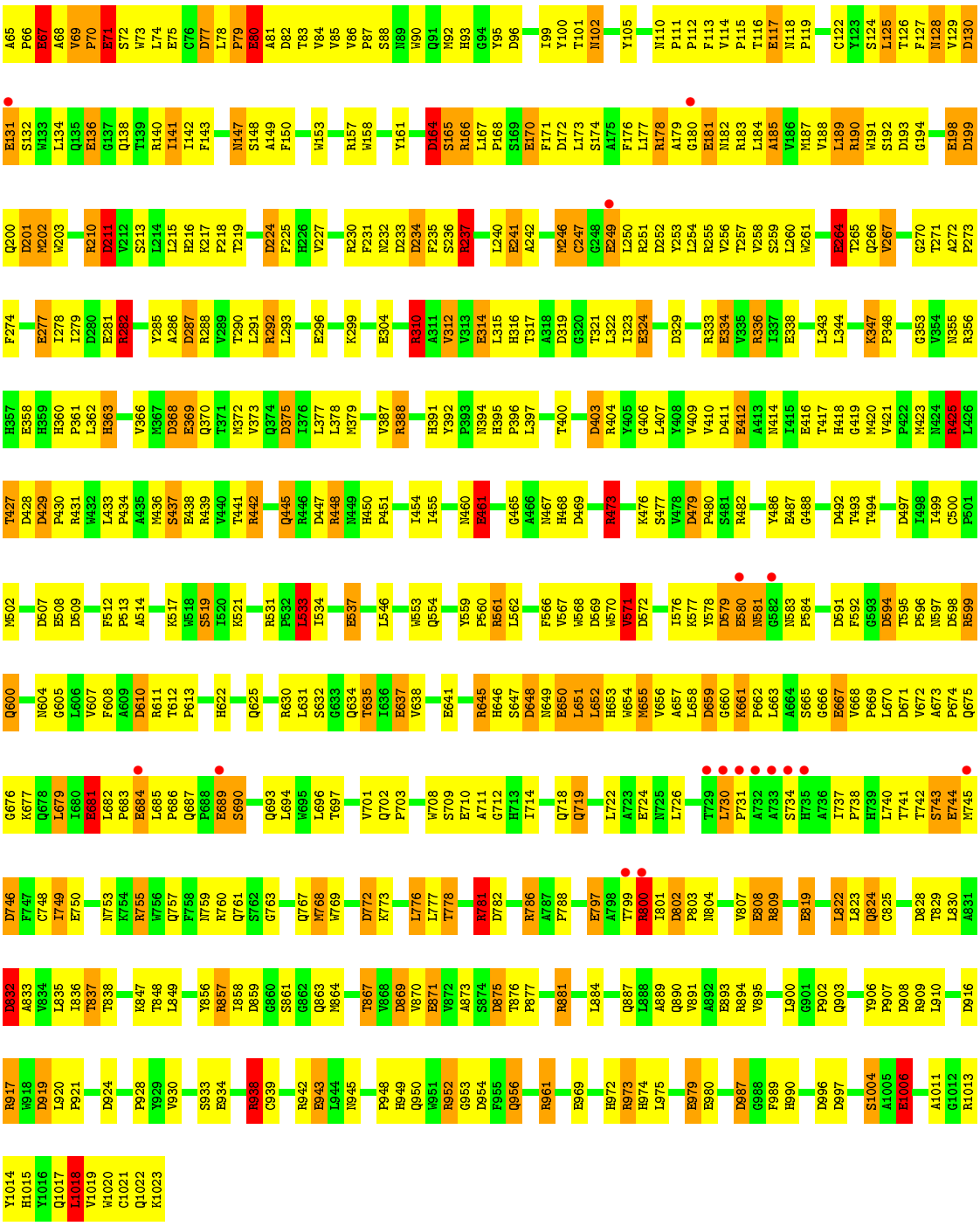
Chain F:



- Molecule 1: Beta-Galactosidase

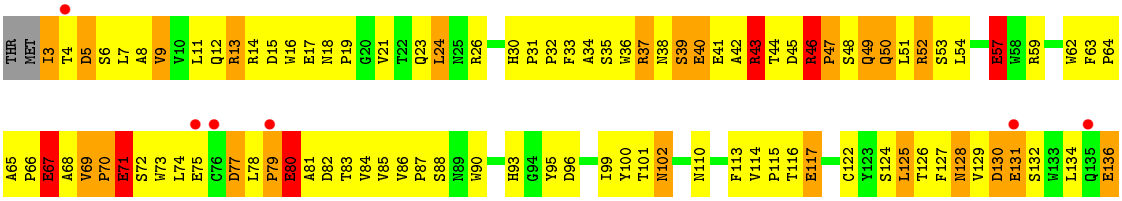
Chain G:

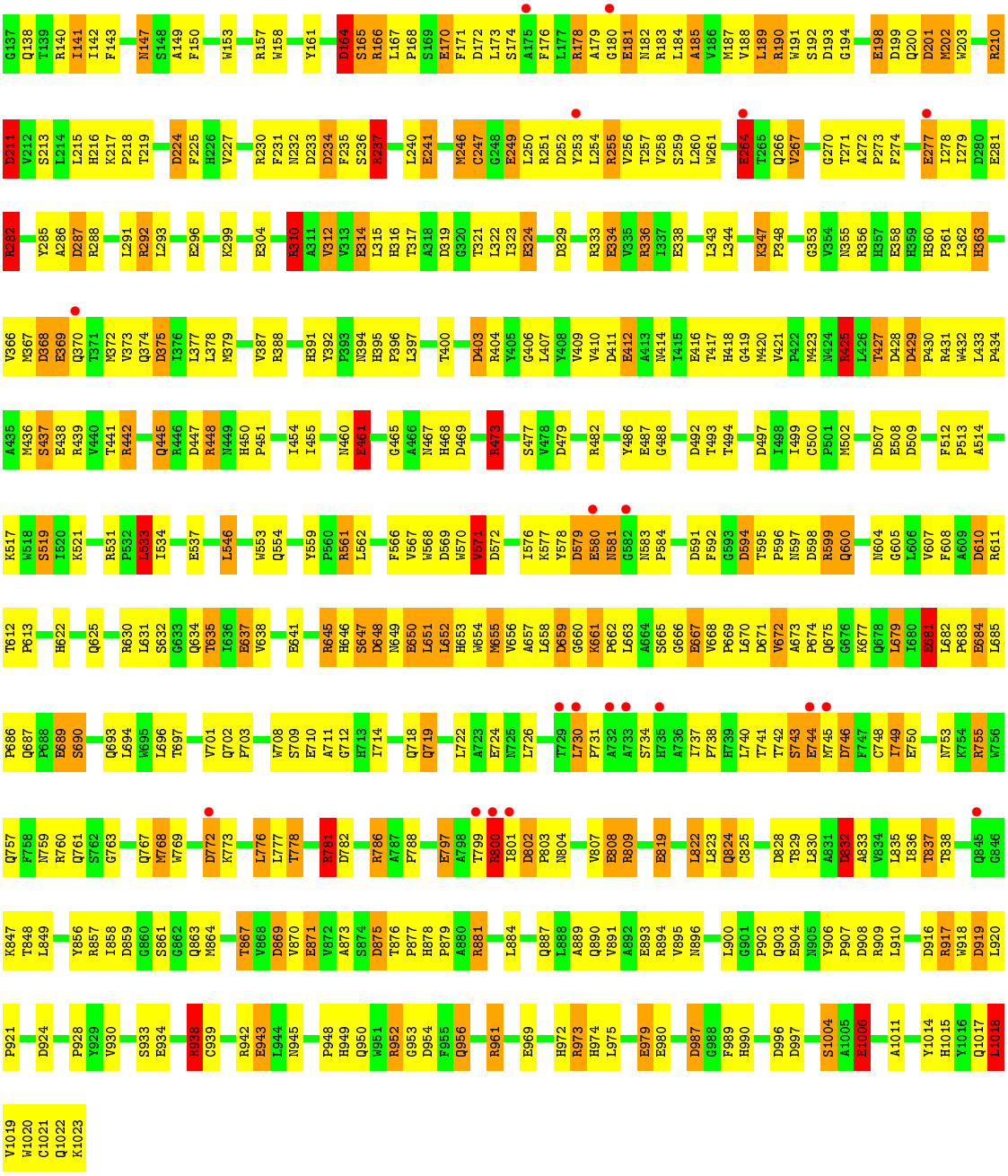




• Molecule 1: Beta-Galactosidase

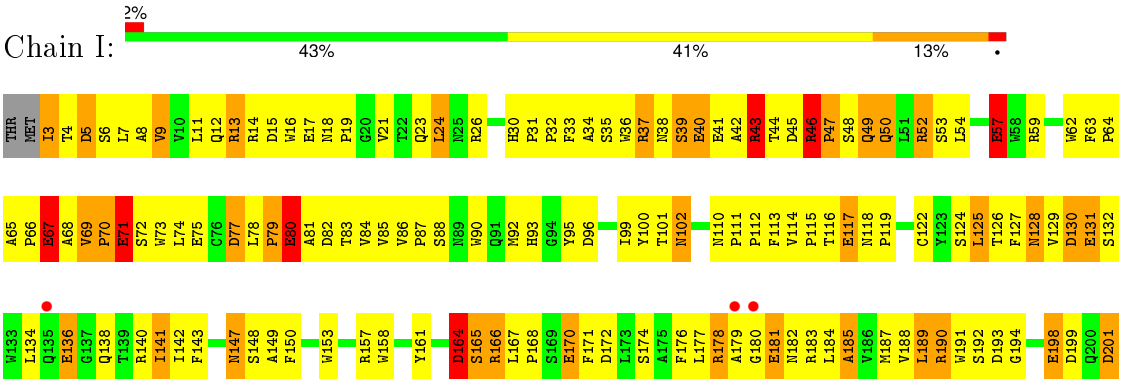
Chain H:

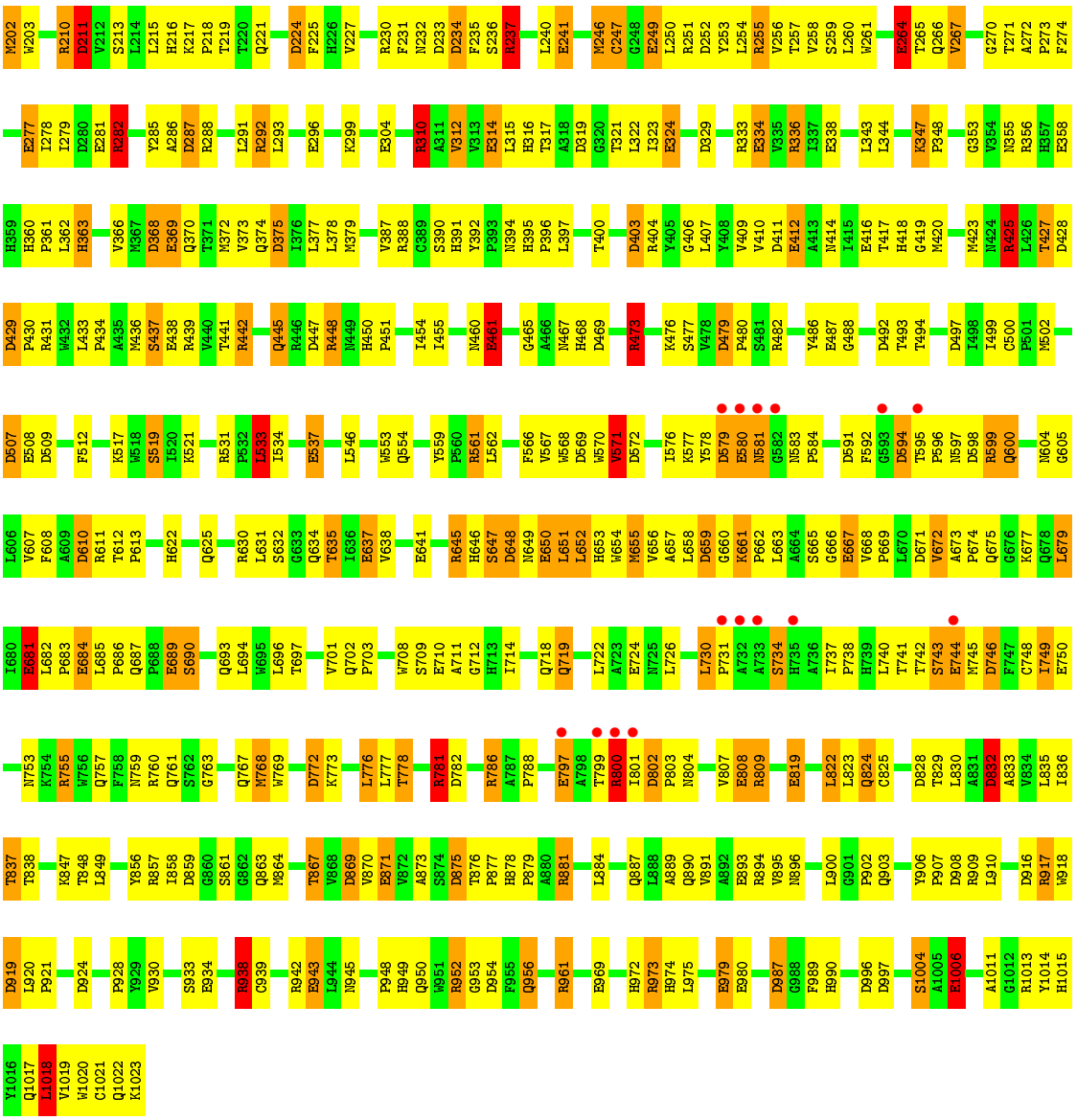




- Molecule 1: Beta-Galactosidase

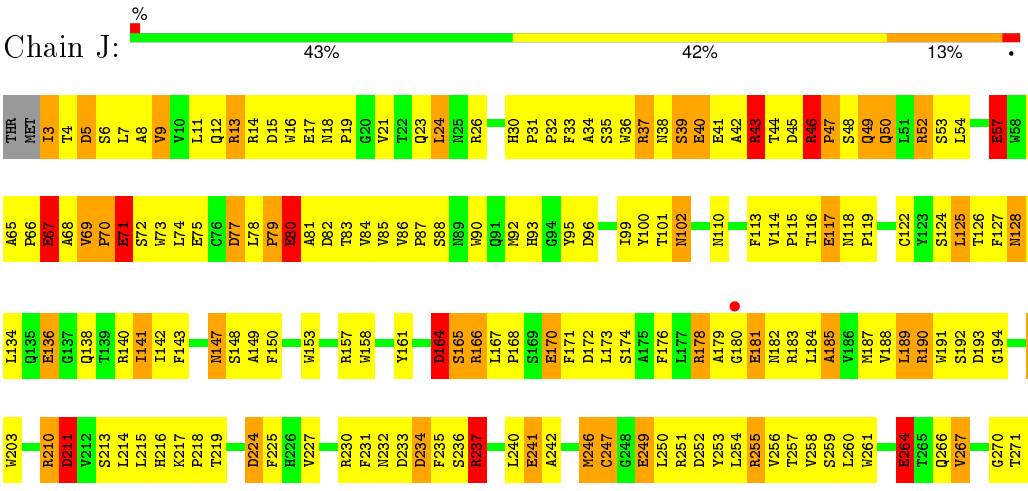
Chain I:

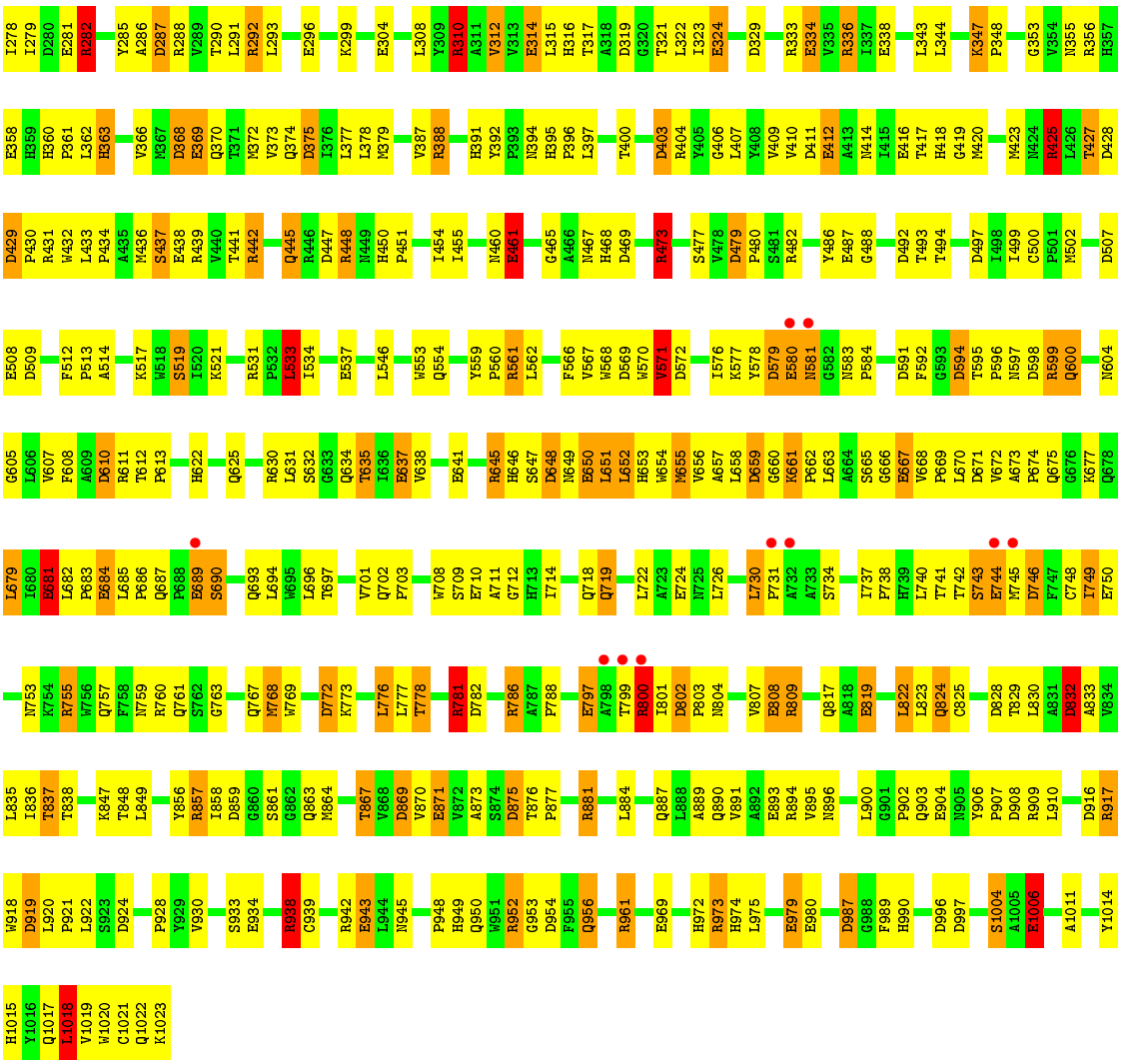




• Molecule 1: Beta-Galactosidase

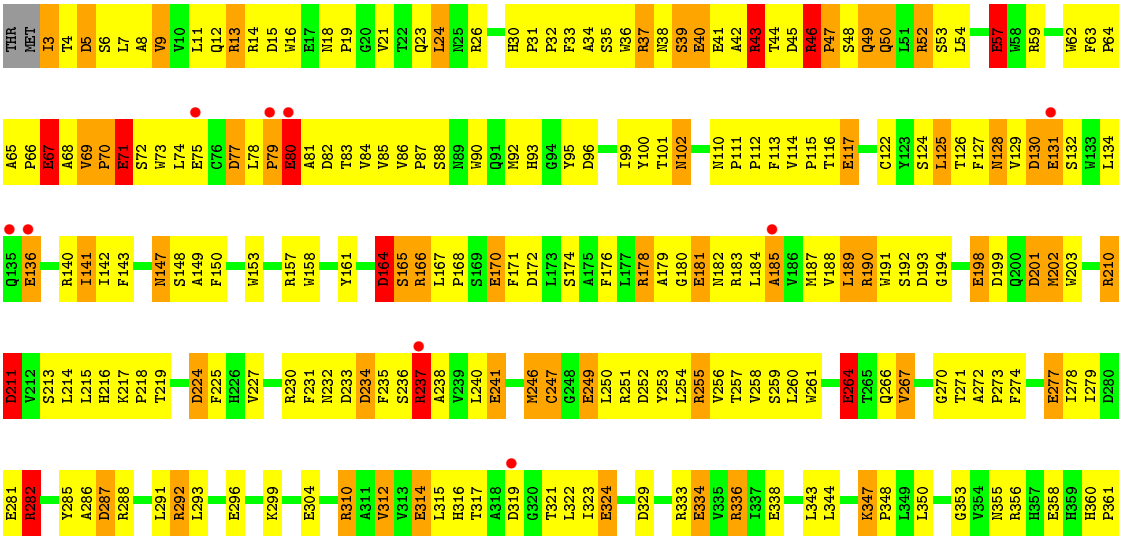
Chain J:

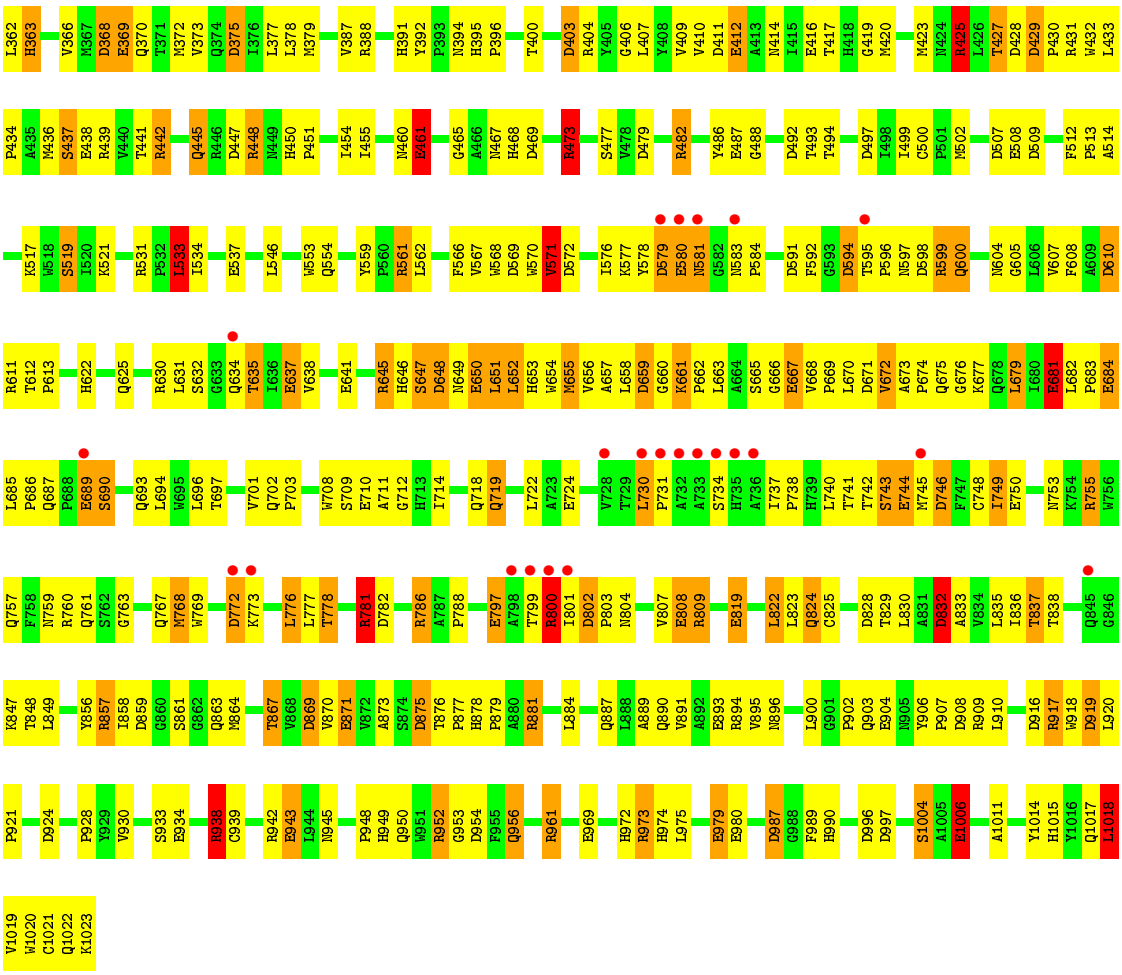




• Molecule 1: Beta-Galactosidase

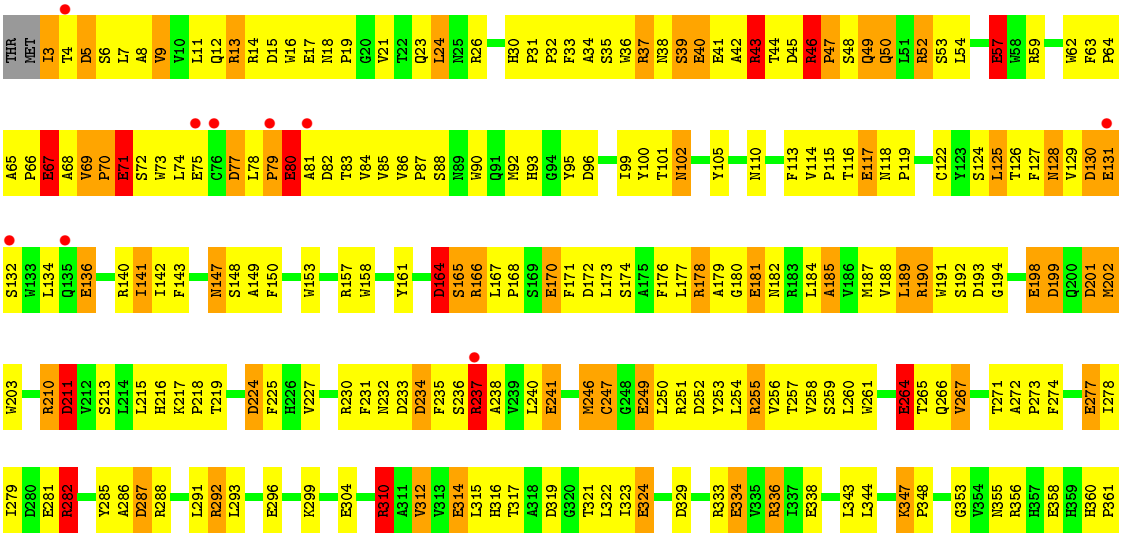
Chain K:

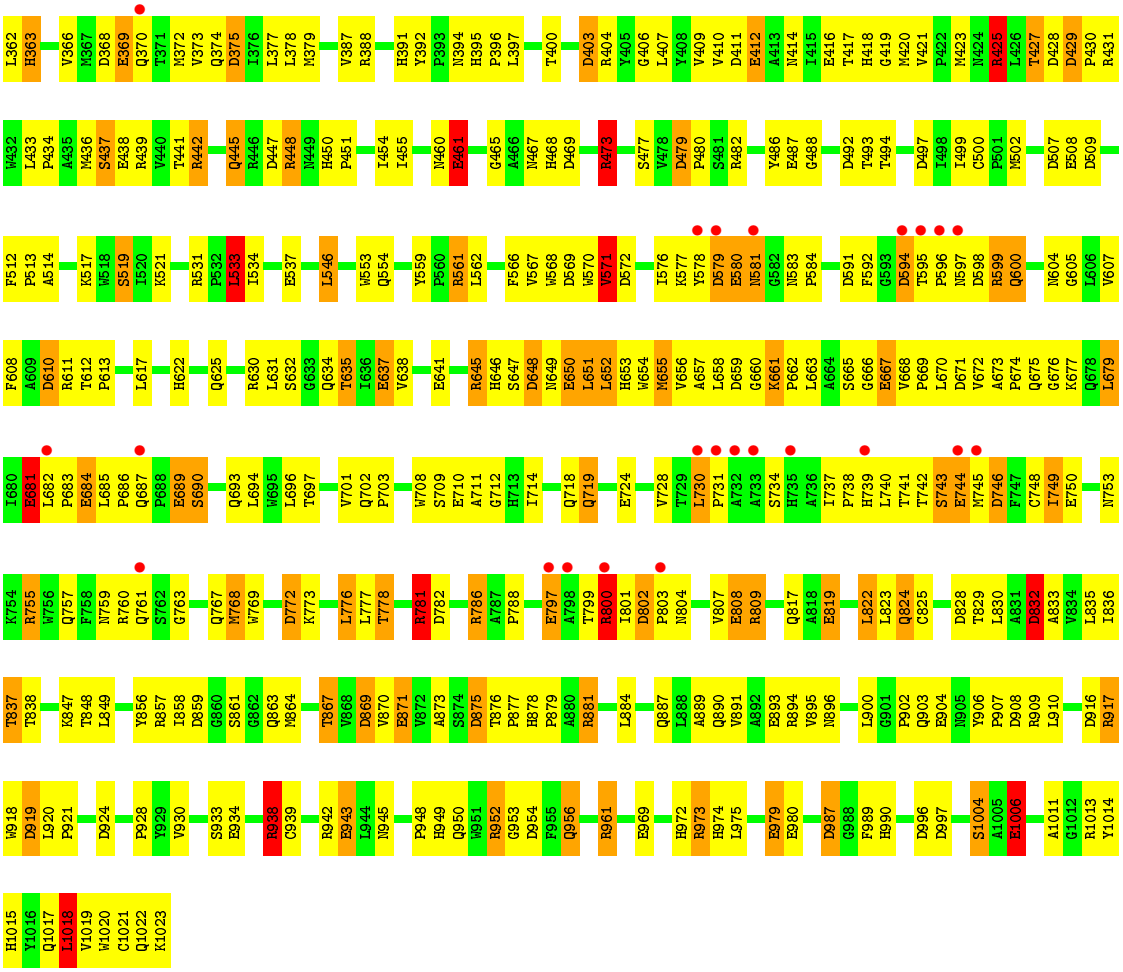




• Molecule 1: Beta-Galactosidase

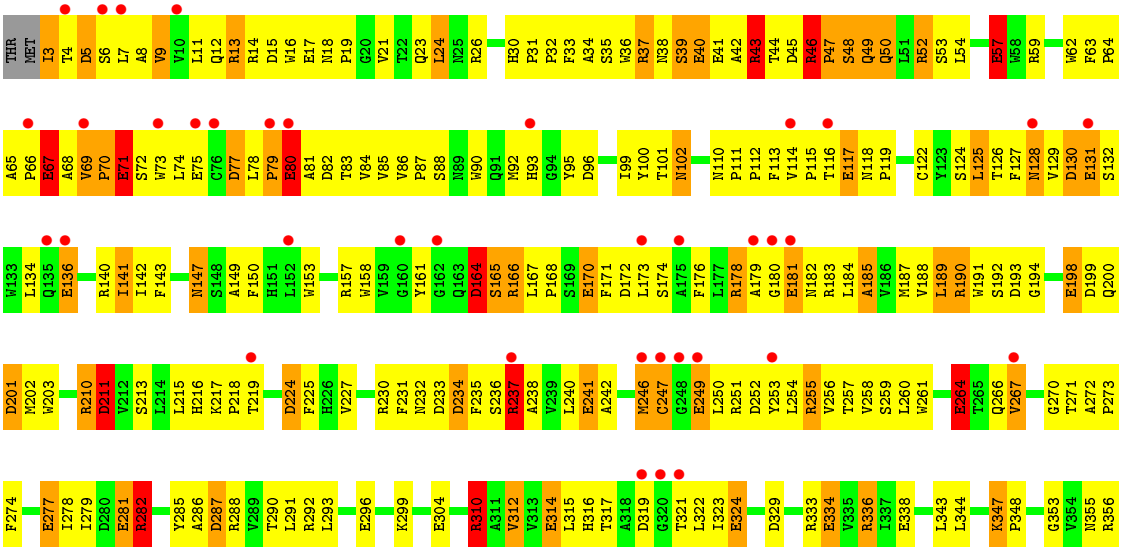
Chain L:

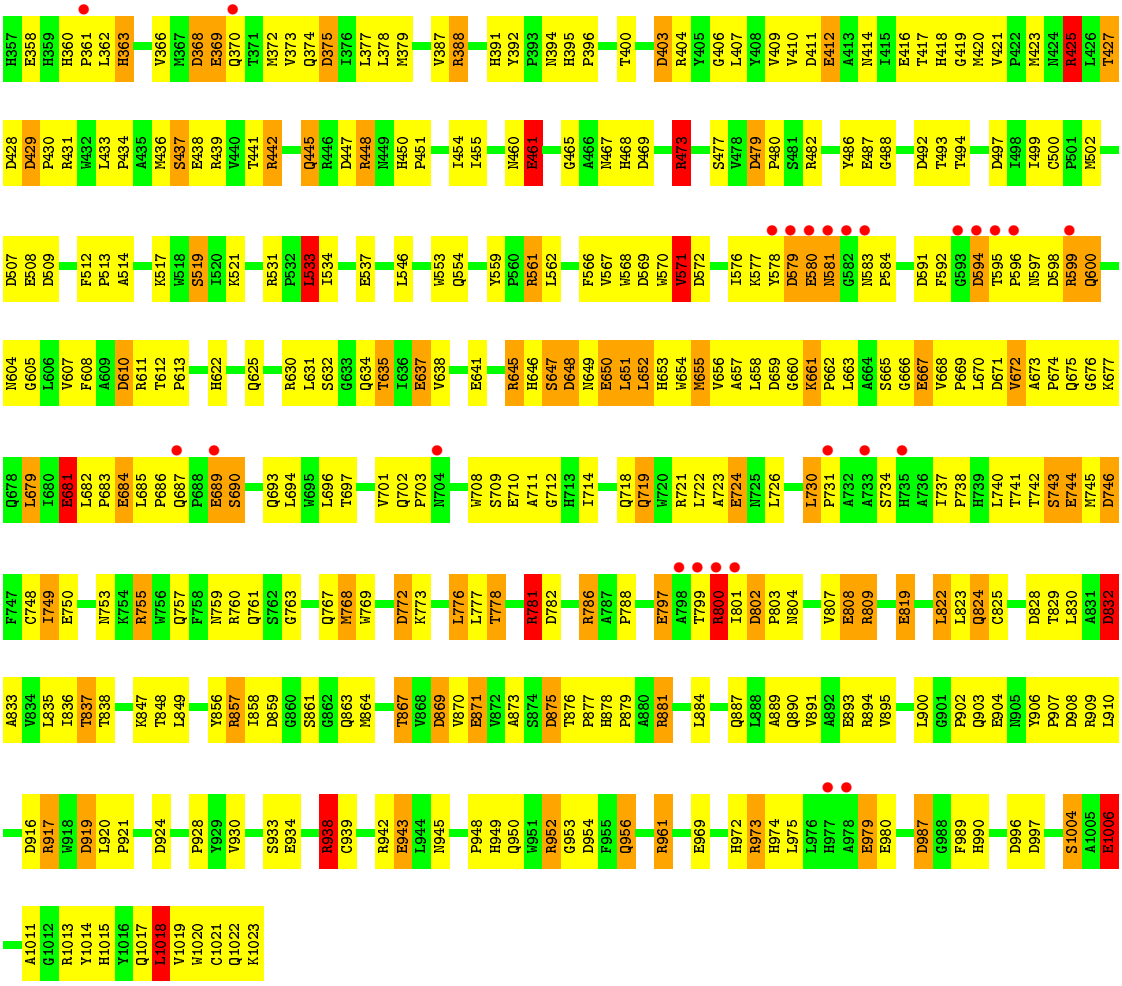




• Molecule 1: Beta-Galactosidase

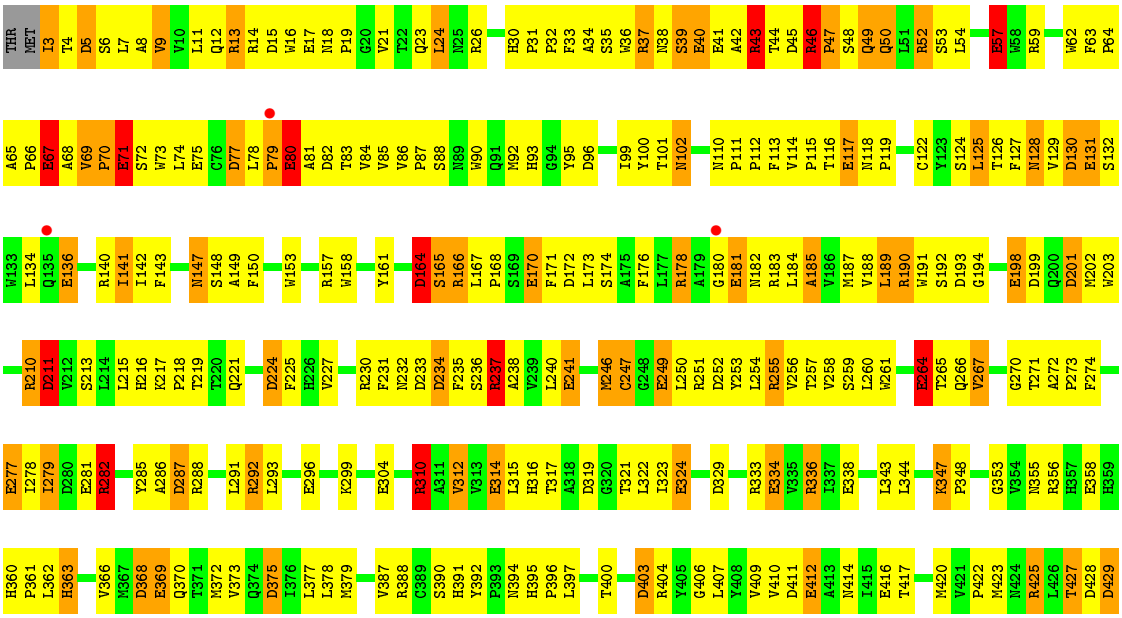
Chain M:



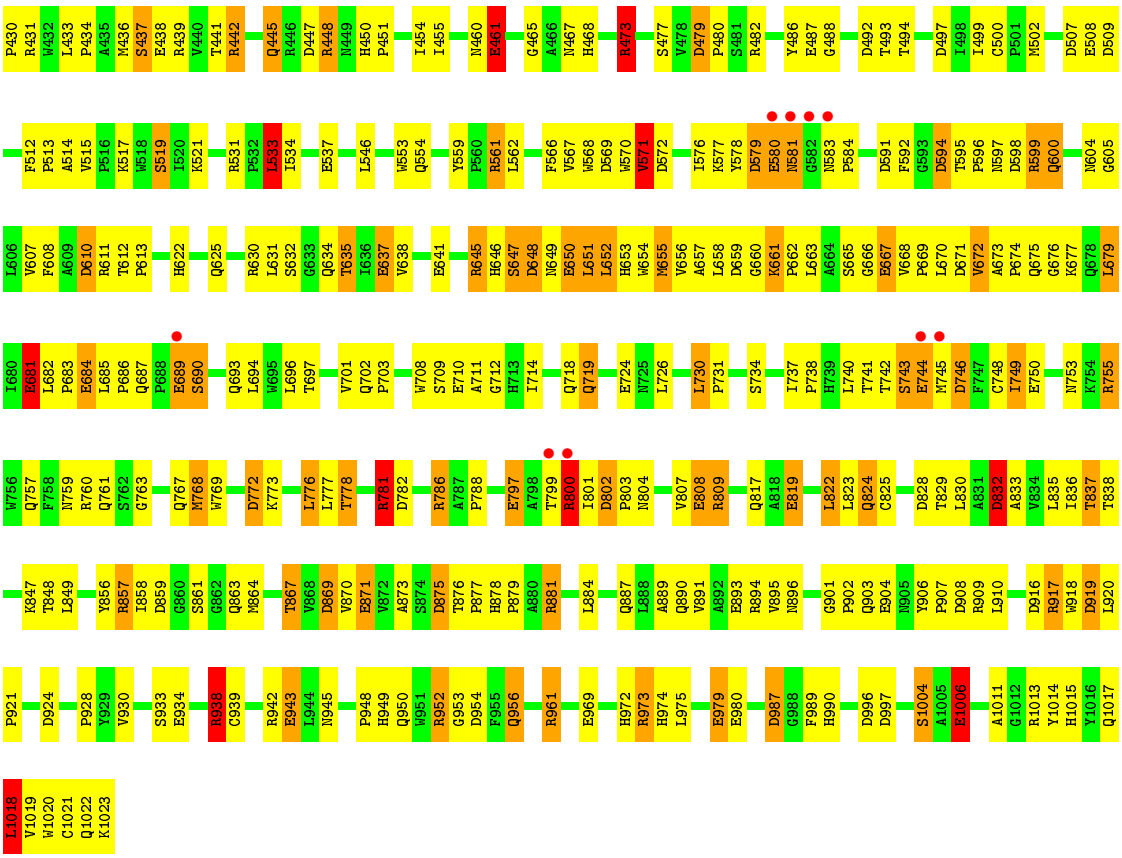


• Molecule 1: Beta-Galactosidase

Chain N:

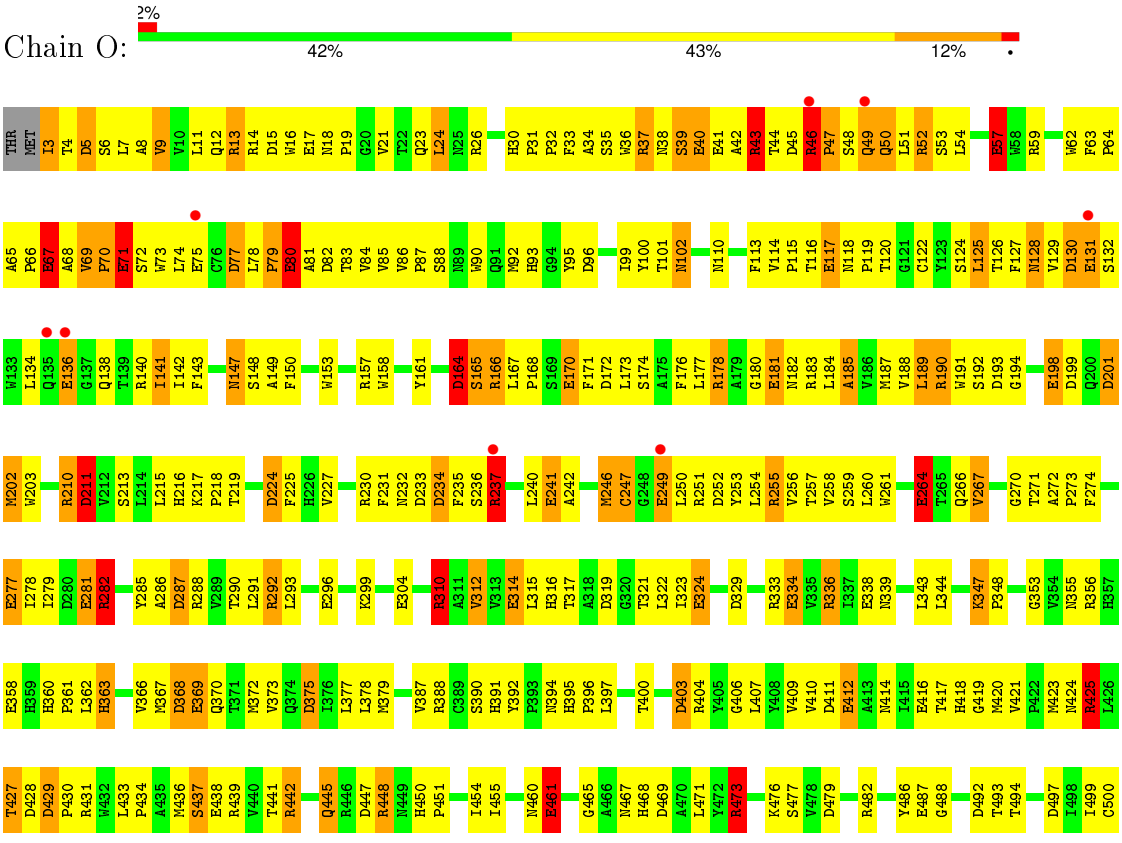


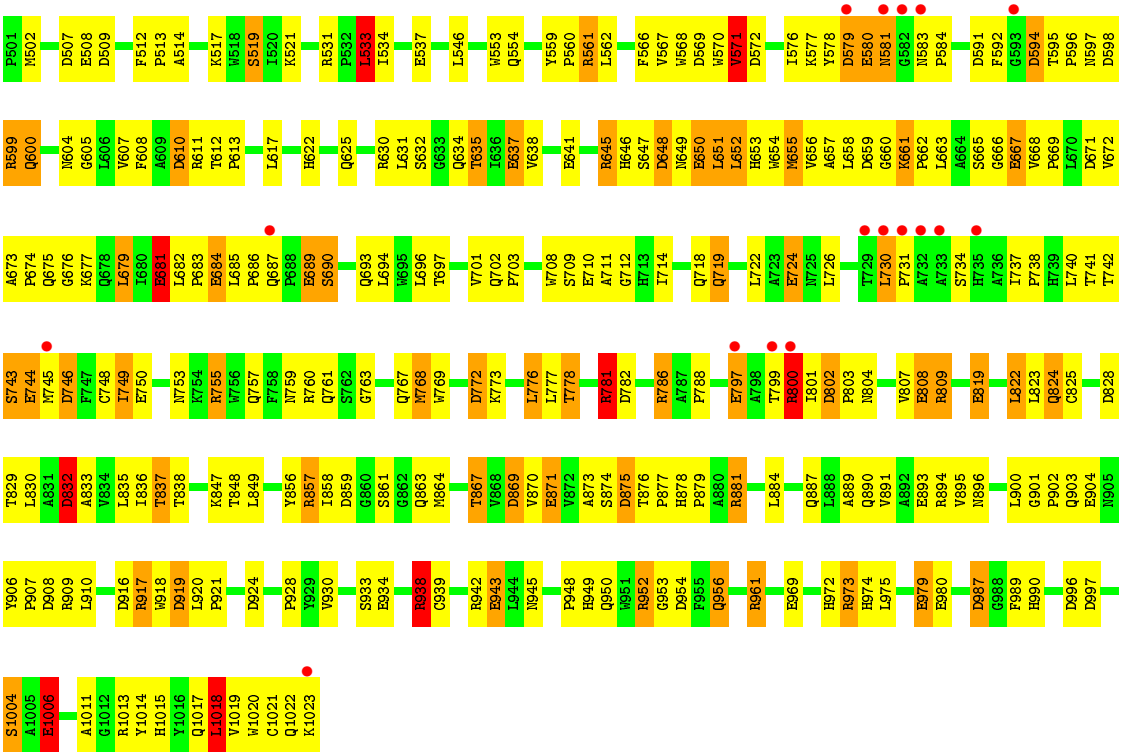
WORLDWIDE PDB PROTEIN DATA BANK



• Molecule 1: Beta-Galactosidase

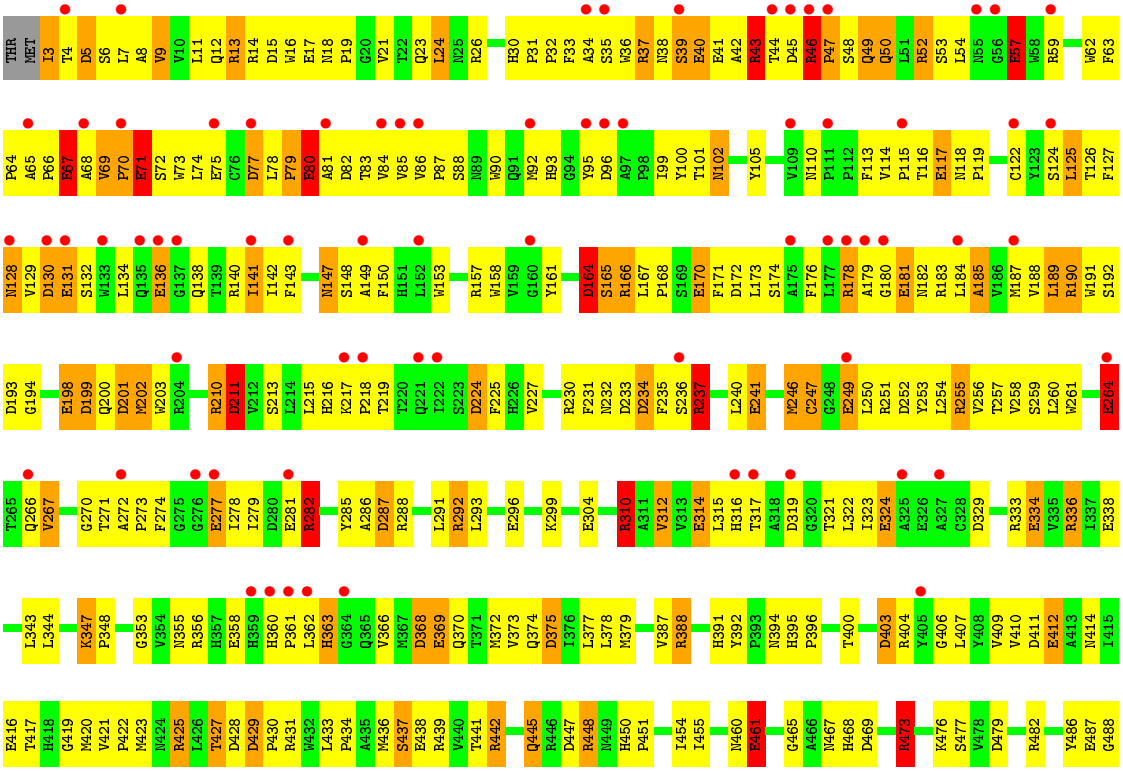
Chain O:

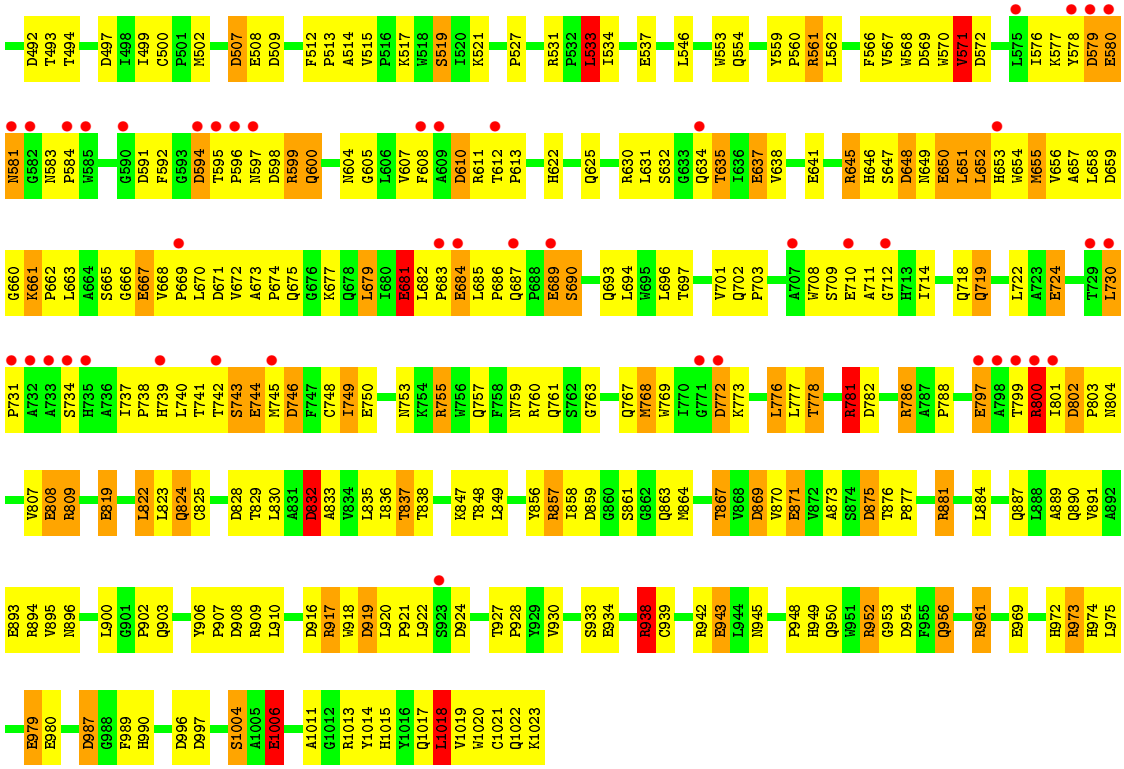




- Molecule 1: Beta-Galactosidase

Chain P:




D492 T493 T494
D497 T498 T499 C500 P501 M502
D507 E508 D509
F512 P513 A514 V515 P516 K517 W518 S519 I520 K521
P527
R531 P532 L533 I534
E537
L546
W553 Q554
Y559 P560 R561 L562
F566 V567 W568 D569 W570 V571 D572
L575 I576 K577 Y578 D579 E580
N581 G582 N583 P584 W585
G590 D591 F592 G593 D594 T595 P596 N597 D598 R599 Q600
N604 G605 L606 V607 F608 A609 D610 R611 T612 P613
H622
Q625
R630 L631 S632 G633 Q634 T635 I636 E637 V638
E641
R645 H646 S647 D648 N649 E650 L651 L652 H653 W654 M655 V656 A657 L658 D659
G660 K661 P662 L663 A664 S665 G666 E667 V668 P669 L670 D671 V672 A673 P674 Q675 G676 K677 Q678 L679 I680 E681 L682 P683 E684 L685 P686 Q687 P688 E689 S690
Q693 L694 W695 L696 T697
V701 Q702 P703
A707 W708 S709 E710 A711 G712 H713 I714
Q718 Q719
L722 A723 E724
T729 L730
P731 A732 A733 S734 H735 A736 I737 P738 H739 L740 T741 T742 S743 E744 W745 D746 F747 C748 I749 E750
N753 K754 R755 W756 Q757 F758 N759 R760 Q761 S762 G763
Q767 N768 W769 I770 G771 D772 K773
L776 L777 T778
R781 D782
R786 A787 P788
E797 A798 T799 R800 I801 D802 P803 N804
V807 E808 R809
E819
L822 L823 Q824 C825
D828 T829 L830 A831 D832 A833 V834 L835 I836 T837 T838
K847 T848 L849
Y856 R857 I858 D859 G860 S861 G862 Q863 M864
T867 V868 D869 V870 E871 V872 A873 S874 D875 T876 P877
R881
L884
Q887 L888 A889 Q890 V891 A892
E893 R894 V895 N896
L900 G901 P902 Q903
Y906 P907 D908 R909 L910
D916 R917 W918 D919 I920 P921 L922 S923 D924
T927 P928 Y929 V930
S933 E934
R938 C939
R942 E943 L944 N945
P948 H949 Q950 W951 R952 G953 D954 F955 Q956
R961
E969
H972 R973 H974 L975
E979 E980
D987 G988 F989 H990
D996 D997
S1004 A1005 E1006
A1011 G1012 R1013 Y1014 H1015 Y1016 Q1017 L1018 V1019 W1020 C1021 Q1022 K1023

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.60Å 207.30Å 510.30Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	66.0 (20.00-2.70) 66.0 (20.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.71Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.234 , (Not available) 0.211 , 0.211	Depositor DCC
R_{free} test set	1854 reflections (0.46%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 79.2	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 409961 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	134528	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% 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, 0.375 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: NA, CME, MG, 2FL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.11	57/8439 (0.7%)	1.47	139/11510 (1.2%)
1	B	1.11	55/8439 (0.7%)	1.47	137/11510 (1.2%)
1	C	1.11	56/8439 (0.7%)	1.47	142/11510 (1.2%)
1	D	1.11	56/8439 (0.7%)	1.47	140/11510 (1.2%)
1	E	1.11	55/8439 (0.7%)	1.47	138/11510 (1.2%)
1	F	1.11	56/8439 (0.7%)	1.47	142/11510 (1.2%)
1	G	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	H	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	I	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	J	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	K	1.11	55/8439 (0.7%)	1.47	139/11510 (1.2%)
1	L	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	M	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	N	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	O	1.11	56/8439 (0.7%)	1.47	140/11510 (1.2%)
1	P	1.11	55/8439 (0.7%)	1.47	143/11510 (1.2%)
All	All	1.11	893/135024 (0.7%)	1.47	2239/184160 (1.2%)

The worst 5 of 893 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	710	GLU	CD-OE2	7.97	1.34	1.25
1	N	710	GLU	CD-OE2	7.97	1.34	1.25
1	A	710	GLU	CD-OE2	7.95	1.34	1.25
1	F	710	GLU	CD-OE2	7.95	1.34	1.25
1	P	710	GLU	CD-OE2	7.94	1.34	1.25

The worst 5 of 2239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	561	ARG	NE-CZ-NH1	10.76	125.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	561	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	I	561	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	C	561	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	D	561	ARG	NE-CZ-NH1	10.68	125.64	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8219	0	7811	586	3
1	B	8219	0	7811	563	5
1	C	8219	0	7811	548	1
1	D	8219	0	7811	585	0
1	E	8219	0	7811	568	0
1	F	8219	0	7811	557	1
1	G	8219	0	7811	571	1
1	H	8219	0	7811	564	0
1	I	8219	0	7811	573	1
1	J	8219	0	7811	566	0
1	K	8219	0	7811	561	0
1	L	8219	0	7811	574	1
1	M	8219	0	7811	566	0
1	N	8219	0	7811	566	0
1	O	8219	0	7811	575	0
1	P	8219	0	7811	576	2
2	A	23	0	21	0	0
2	B	23	0	21	0	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	A	160	0	0	6	0
5	B	163	0	0	6	0
5	C	162	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	163	0	0	6	0
5	E	162	0	0	6	0
5	F	162	0	0	6	0
5	G	162	0	0	6	0
5	H	162	0	0	6	0
5	I	162	0	0	6	1
5	J	162	0	0	6	0
5	K	162	0	0	6	0
5	L	162	0	0	6	0
5	M	161	0	0	6	0
5	N	163	0	0	6	0
5	O	161	0	0	6	0
5	P	163	0	0	6	0
All	All	134528	0	125312	8966	8

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 35.

The worst 5 of 8966 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:J:43:ARG:HH11	1:J:43:ARG:HG2	1.20	1.07
1:H:43:ARG:HG2	1:H:43:ARG:HH11	1.20	1.07
1:I:43:ARG:HH11	1:I:43:ARG:HG2	1.20	1.07
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.20	1.07
1:M:43:ARG:HH11	1:M:43:ARG:HG2	1.20	1.06

The worst 5 of 8 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:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.57	0.63
1:A:580:GLU:O	1:B:578:TYR:CB[2_555]	1.68	0.52
1:G:740:LEU:O	1:L:739:HIS:CD2[1_455]	1.94	0.26
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	1.97	0.23
1:B:740:LEU:O	1:P:739:HIS:CD2[1_354]	2.09	0.11

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	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	B	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	C	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	D	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	E	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	F	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	G	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	H	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	I	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	J	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	K	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	L	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	M	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	N	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	O	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
1	P	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	21	49
All	All	16288/16368 (100%)	15296 (94%)	848 (5%)	144 (1%)	21	49

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	B	174	SER
1	C	174	SER
1	D	174	SER
1	E	174	SER

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	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	B	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	C	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	D	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	E	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	F	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	G	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	H	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	I	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	J	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	K	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	L	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	M	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	N	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	O	872/872 (100%)	759 (87%)	113 (13%)	5	12
1	P	872/872 (100%)	759 (87%)	113 (13%)	5	12
All	All	13952/13952 (100%)	12144 (87%)	1808 (13%)	5	12

5 of 1808 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	165	SER
1	I	938	ARG
1	O	768	MET
1	H	347	LYS
1	I	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	316	HIS
1	I	1017	GLN
1	O	761	GLN
1	H	467	ASN
1	I	128	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

48 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	A	1021	1	8,9,10	0.59	0	6,9,11	1.34	0
1	CME	A	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	A	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	B	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	B	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	B	914	1	8,9,10	0.80	0	6,9,11	2.06	1 (16%)
1	CME	C	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	C	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	C	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	D	1021	1	8,9,10	0.61	0	6,9,11	1.33	0
1	CME	D	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	D	914	1	8,9,10	0.80	0	6,9,11	2.05	1 (16%)
1	CME	E	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	E	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	E	914	1	8,9,10	0.81	0	6,9,11	2.06	1 (16%)
1	CME	F	1021	1	8,9,10	0.61	0	6,9,11	1.33	0
1	CME	F	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CME	F	914	1	8,9,10	0.80	0	6,9,11	2.06	1 (16%)
1	CME	G	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	G	748	1	8,9,10	0.81	0	6,9,11	1.64	2 (33%)
1	CME	G	914	1	8,9,10	0.81	0	6,9,11	2.06	1 (16%)
1	CME	H	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	H	748	1	8,9,10	0.80	0	6,9,11	1.65	2 (33%)
1	CME	H	914	1	8,9,10	0.80	0	6,9,11	2.05	1 (16%)
1	CME	I	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	I	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	I	914	1	8,9,10	0.80	0	6,9,11	2.06	1 (16%)
1	CME	J	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	J	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	J	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	K	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	K	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	K	914	1	8,9,10	0.81	0	6,9,11	2.06	1 (16%)
1	CME	L	1021	1	8,9,10	0.60	0	6,9,11	1.34	0
1	CME	L	748	1	8,9,10	0.81	0	6,9,11	1.64	2 (33%)
1	CME	L	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	M	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	M	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	M	914	1	8,9,10	0.81	0	6,9,11	2.06	1 (16%)
1	CME	N	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	N	748	1	8,9,10	0.81	0	6,9,11	1.64	2 (33%)
1	CME	N	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	O	1021	1	8,9,10	0.60	0	6,9,11	1.34	0
1	CME	O	748	1	8,9,10	0.81	0	6,9,11	1.65	2 (33%)
1	CME	O	914	1	8,9,10	0.81	0	6,9,11	2.05	1 (16%)
1	CME	P	1021	1	8,9,10	0.60	0	6,9,11	1.33	0
1	CME	P	748	1	8,9,10	0.82	0	6,9,11	1.65	2 (33%)
1	CME	P	914	1	8,9,10	0.81	0	6,9,11	2.06	1 (16%)

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
1	CME	A	1021	1	-	0/5/8/10	0/0/0/0
1	CME	A	748	1	-	0/5/8/10	0/0/0/0
1	CME	A	914	1	-	0/5/8/10	0/0/0/0
1	CME	B	1021	1	-	0/5/8/10	0/0/0/0
1	CME	B	748	1	-	0/5/8/10	0/0/0/0
1	CME	B	914	1	-	0/5/8/10	0/0/0/0
1	CME	C	1021	1	-	0/5/8/10	0/0/0/0
1	CME	C	748	1	-	0/5/8/10	0/0/0/0
1	CME	C	914	1	-	0/5/8/10	0/0/0/0
1	CME	D	1021	1	-	0/5/8/10	0/0/0/0
1	CME	D	748	1	-	0/5/8/10	0/0/0/0
1	CME	D	914	1	-	0/5/8/10	0/0/0/0
1	CME	E	1021	1	-	0/5/8/10	0/0/0/0
1	CME	E	748	1	-	0/5/8/10	0/0/0/0
1	CME	E	914	1	-	0/5/8/10	0/0/0/0
1	CME	F	1021	1	-	0/5/8/10	0/0/0/0
1	CME	F	748	1	-	0/5/8/10	0/0/0/0
1	CME	F	914	1	-	0/5/8/10	0/0/0/0
1	CME	G	1021	1	-	0/5/8/10	0/0/0/0
1	CME	G	748	1	-	0/5/8/10	0/0/0/0
1	CME	G	914	1	-	0/5/8/10	0/0/0/0
1	CME	H	1021	1	-	0/5/8/10	0/0/0/0
1	CME	H	748	1	-	0/5/8/10	0/0/0/0
1	CME	H	914	1	-	0/5/8/10	0/0/0/0
1	CME	I	1021	1	-	0/5/8/10	0/0/0/0
1	CME	I	748	1	-	0/5/8/10	0/0/0/0
1	CME	I	914	1	-	0/5/8/10	0/0/0/0
1	CME	J	1021	1	-	0/5/8/10	0/0/0/0
1	CME	J	748	1	-	0/5/8/10	0/0/0/0
1	CME	J	914	1	-	0/5/8/10	0/0/0/0
1	CME	K	1021	1	-	0/5/8/10	0/0/0/0
1	CME	K	748	1	-	0/5/8/10	0/0/0/0
1	CME	K	914	1	-	0/5/8/10	0/0/0/0
1	CME	L	1021	1	-	0/5/8/10	0/0/0/0
1	CME	L	748	1	-	0/5/8/10	0/0/0/0
1	CME	L	914	1	-	0/5/8/10	0/0/0/0
1	CME	M	1021	1	-	0/5/8/10	0/0/0/0
1	CME	M	748	1	-	0/5/8/10	0/0/0/0
1	CME	M	914	1	-	0/5/8/10	0/0/0/0
1	CME	N	1021	1	-	0/5/8/10	0/0/0/0
1	CME	N	748	1	-	0/5/8/10	0/0/0/0
1	CME	N	914	1	-	0/5/8/10	0/0/0/0
1	CME	O	1021	1	-	0/5/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	O	748	1	-	0/5/8/10	0/0/0/0
1	CME	O	914	1	-	0/5/8/10	0/0/0/0
1	CME	P	1021	1	-	0/5/8/10	0/0/0/0
1	CME	P	748	1	-	0/5/8/10	0/0/0/0
1	CME	P	914	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	914	CME	CB-SG-SD	-4.62	94.94	103.95
1	I	914	CME	CB-SG-SD	-4.62	94.95	103.95
1	E	914	CME	CB-SG-SD	-4.62	94.95	103.95
1	K	914	CME	CB-SG-SD	-4.62	94.95	103.95
1	F	914	CME	CB-SG-SD	-4.62	94.95	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1021	CME	7	0
1	A	748	CME	2	0
1	B	1021	CME	7	0
1	B	748	CME	2	0
1	C	1021	CME	6	0
1	C	748	CME	2	0
1	D	1021	CME	6	0
1	D	748	CME	2	0
1	E	1021	CME	7	0
1	E	748	CME	2	0
1	F	1021	CME	6	0
1	F	748	CME	2	0
1	G	1021	CME	7	0
1	G	748	CME	2	0
1	H	1021	CME	6	0
1	H	748	CME	2	0
1	I	1021	CME	7	0
1	I	748	CME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	1021	CME	7	0
1	J	748	CME	2	0
1	K	1021	CME	6	0
1	K	748	CME	2	0
1	L	1021	CME	6	0
1	L	748	CME	2	0
1	M	1021	CME	6	0
1	M	748	CME	2	0
1	N	1021	CME	7	0
1	N	748	CME	2	0
1	O	1021	CME	7	0
1	O	748	CME	2	0
1	P	1021	CME	6	0
1	P	748	CME	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 80 ligands modelled in this entry, 64 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	2FL	A	2001	4	23,24,24	0.55	0	33,35,35	1.44	2 (6%)
2	2FL	B	2001	4	23,24,24	0.54	0	33,35,35	1.43	2 (6%)
2	2FL	C	2001	4	23,24,24	0.55	0	33,35,35	1.44	2 (6%)
2	2FL	D	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	E	2001	4	23,24,24	0.55	0	33,35,35	1.43	1 (3%)
2	2FL	F	2001	4	23,24,24	0.56	0	33,35,35	1.42	2 (6%)
2	2FL	G	2001	4	23,24,24	0.56	0	33,35,35	1.43	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	2FL	H	2001	4	23,24,24	0.55	0	33,35,35	1.44	2 (6%)
2	2FL	I	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	J	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	K	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	L	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	M	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	N	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)
2	2FL	O	2001	4	23,24,24	0.54	0	33,35,35	1.43	2 (6%)
2	2FL	P	2001	4	23,24,24	0.55	0	33,35,35	1.43	2 (6%)

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	2FL	A	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	B	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	C	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	D	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	E	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	F	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	G	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	H	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	I	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	J	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	K	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	L	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	M	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	N	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	O	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	P	2001	4	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	2001	2FL	C1-C2-C3	2.00	114.61	111.52
2	F	2001	2FL	C1-C2-C3	2.00	114.61	111.52
2	D	2001	2FL	C1-C2-C3	2.00	114.61	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	2FL	C1-C2-C3	2.01	114.62	111.52
2	H	2001	2FL	C1-C2-C3	2.01	114.62	111.52

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1018/1023 (99%)	-0.61	13 (1%) 79 79	2, 23, 63, 99	0
1	B	1018/1023 (99%)	-0.61	10 (0%) 84 85	1, 21, 61, 98	0
1	C	1018/1023 (99%)	-0.62	9 (0%) 85 86	1, 21, 61, 98	0
1	D	1018/1023 (99%)	-0.39	15 (1%) 76 76	10, 31, 69, 100	0
1	E	1018/1023 (99%)	0.14	38 (3%) 45 45	27, 48, 83, 100	0
1	F	1018/1023 (99%)	-0.53	8 (0%) 87 88	8, 28, 67, 100	0
1	G	1018/1023 (99%)	-0.46	17 (1%) 73 74	8, 28, 68, 100	0
1	H	1018/1023 (99%)	-0.14	26 (2%) 59 59	18, 38, 75, 100	0
1	I	1018/1023 (99%)	-0.35	18 (1%) 71 72	11, 32, 70, 100	0
1	J	1018/1023 (99%)	-0.50	11 (1%) 82 83	10, 30, 69, 100	0
1	K	1018/1023 (99%)	-0.12	32 (3%) 52 52	24, 45, 81, 100	0
1	L	1018/1023 (99%)	-0.07	32 (3%) 52 52	25, 45, 81, 100	0
1	M	1018/1023 (99%)	0.35	62 (6%) 25 23	27, 48, 83, 100	0
1	N	1018/1023 (99%)	-0.32	12 (1%) 81 81	16, 36, 74, 100	0
1	O	1018/1023 (99%)	-0.21	25 (2%) 61 61	21, 42, 78, 100	0
1	P	1018/1023 (99%)	0.81	117 (11%) 6 5	39, 60, 91, 100	0
All	All	16288/16368 (99%)	-0.23	445 (2%) 58 58	1, 37, 76, 100	0

The worst 5 of 445 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	799	THR	6.4
1	G	735	HIS	6.3
1	F	581	ASN	6.1
1	G	732	ALA	5.9
1	K	735	HIS	5.9

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	H	914	10/11	0.95	0.15	-	33,40,77,82	0
1	CME	H	748	10/11	0.92	0.21	-	46,58,92,100	0
1	CME	E	1021	10/11	0.88	0.20	-	60,76,100,100	0
1	CME	J	914	10/11	0.96	0.14	-	25,32,69,75	0
1	CME	L	914	10/11	0.94	0.15	-	40,47,84,89	0
1	CME	C	1021	10/11	0.90	0.15	-	33,49,84,97	0
1	CME	K	748	10/11	0.91	0.19	-	53,65,98,100	0
1	CME	A	1021	10/11	0.89	0.19	-	35,50,85,99	0
1	CME	F	1021	10/11	0.89	0.17	-	40,56,91,100	0
1	CME	P	914	10/11	0.84	0.22	-	54,62,98,100	0
1	CME	J	1021	10/11	0.87	0.22	-	42,58,93,100	0
1	CME	C	748	10/11	0.92	0.19	-	29,41,74,86	0
1	CME	A	748	10/11	0.93	0.19	-	31,43,76,87	0
1	CME	J	748	10/11	0.92	0.16	-	38,50,84,95	0
1	CME	B	748	10/11	0.92	0.17	-	29,41,75,86	0
1	CME	E	914	10/11	0.92	0.19	-	42,50,87,92	0
1	CME	I	748	10/11	0.92	0.17	-	40,52,85,97	0
1	CME	D	1021	10/11	0.91	0.19	-	43,58,93,100	0
1	CME	K	1021	10/11	0.90	0.21	-	57,73,100,100	0
1	CME	H	1021	10/11	0.87	0.20	-	50,66,100,100	0
1	CME	D	914	10/11	0.96	0.14	-	25,33,69,75	0
1	CME	L	748	10/11	0.90	0.20	-	53,65,99,100	0
1	CME	E	748	10/11	0.93	0.25	-	56,68,100,100	0
1	CME	N	1021	10/11	0.87	0.18	-	48,64,99,100	0
1	CME	M	914	10/11	0.91	0.16	-	42,50,86,92	0
1	CME	F	748	10/11	0.92	0.19	-	36,48,81,93	0
1	CME	O	914	10/11	0.95	0.13	-	36,44,80,86	0
1	CME	I	914	10/11	0.95	0.13	-	26,34,70,76	0
1	CME	O	748	10/11	0.86	0.33	-	50,62,95,100	0
1	CME	B	1021	10/11	0.87	0.25	-	33,49,84,97	0
1	CME	G	1021	10/11	0.93	0.17	-	41,56,91,100	0
1	CME	A	914	10/11	0.94	0.17	-	17,25,61,67	0
1	CME	F	914	10/11	0.96	0.13	-	23,30,67,72	0
1	CME	O	1021	10/11	0.92	0.21	-	54,69,100,100	0
1	CME	P	1021	10/11	0.81	0.32	-	72,87,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	N	748	10/11	0.91	0.24	-	44,56,90,100	0
1	CME	L	1021	10/11	0.88	0.16	-	57,73,100,100	0
1	CME	N	914	10/11	0.97	0.12	-	31,38,75,81	0
1	CME	G	914	10/11	0.96	0.10	-	23,31,67,73	0
1	CME	I	1021	10/11	0.94	0.15	-	44,60,94,100	0
1	CME	D	748	10/11	0.92	0.20	-	39,51,84,95	0
1	CME	K	914	10/11	0.94	0.12	-	40,47,84,89	0
1	CME	M	1021	10/11	0.90	0.17	-	60,75,100,100	0
1	CME	B	914	10/11	0.96	0.12	-	16,23,60,66	0
1	CME	G	748	10/11	0.91	0.18	-	37,48,82,93	0
1	CME	M	748	10/11	0.89	0.26	-	56,68,100,100	0
1	CME	P	748	10/11	0.85	0.25	-	68,80,100,100	0
1	CME	C	914	10/11	0.97	0.10	-	16,23,60,65	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	G	2002	1/1	0.96	0.27	8.68	29,29,29,29	0
3	MG	B	2002	1/1	0.99	0.23	8.55	22,22,22,22	0
4	NA	E	2004	1/1	0.82	0.37	6.47	55,55,55,55	0
3	MG	F	2002	1/1	0.98	0.22	5.77	29,29,29,29	0
2	2FL	K	2001	23/23	0.86	0.27	5.56	63,74,91,100	0
2	2FL	O	2001	23/23	0.85	0.24	5.27	59,70,87,100	0
4	NA	O	2005	1/1	0.86	0.16	4.77	37,37,37,37	0
3	MG	C	2002	1/1	0.95	0.22	4.69	22,22,22,22	0
4	NA	M	2004	1/1	0.72	0.32	4.66	55,55,55,55	0
3	MG	N	2002	1/1	0.98	0.19	4.48	37,37,37,37	0
4	NA	J	2004	1/1	0.85	0.20	4.44	38,38,38,38	0
2	2FL	H	2001	23/23	0.84	0.28	4.33	56,67,84,100	0
3	MG	O	2002	1/1	0.98	0.25	4.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	H	2002	1/1	0.97	0.26	3.93	39,39,39,39	0
4	NA	F	2005	1/1	0.89	0.13	3.83	23,23,23,23	0
2	2FL	G	2001	23/23	0.91	0.18	3.79	46,57,74,97	0
4	NA	N	2005	1/1	0.98	0.16	3.55	31,31,31,31	0
4	NA	J	2005	1/1	0.91	0.17	3.53	25,25,25,25	0
2	2FL	F	2001	23/23	0.90	0.19	3.51	46,57,74,96	0
2	2FL	L	2001	23/23	0.84	0.29	3.47	63,74,91,100	0
4	NA	P	2004	1/1	0.40	0.36	3.33	67,67,67,67	0
2	2FL	J	2001	23/23	0.89	0.21	3.13	48,59,76,99	0
4	NA	B	2005	1/1	0.95	0.12	3.05	16,16,16,16	0
2	2FL	C	2001	23/23	0.88	0.21	2.99	39,50,67,89	0
2	2FL	B	2001	23/23	0.91	0.16	2.84	39,50,67,90	0
4	NA	K	2004	1/1	0.90	0.21	2.77	53,53,53,53	0
2	2FL	E	2001	23/23	0.90	0.21	2.38	66,77,94,100	0
3	MG	I	2002	1/1	0.98	0.22	2.35	32,32,32,32	0
2	2FL	D	2001	23/23	0.93	0.21	2.21	48,60,76,99	0
3	MG	D	2002	1/1	0.95	0.18	2.09	31,31,31,31	0
4	NA	L	2004	1/1	0.83	0.25	2.06	53,53,53,53	0
2	2FL	A	2001	23/23	0.91	0.16	1.83	40,52,68,91	0
2	2FL	N	2001	23/23	0.92	0.17	1.61	54,65,82,100	0
3	MG	E	2002	1/1	0.96	0.21	1.56	48,48,48,48	0
3	MG	L	2002	1/1	0.95	0.20	1.25	46,46,46,46	0
4	NA	L	2005	1/1	0.95	0.15	1.10	40,40,40,40	0
4	NA	O	2004	1/1	0.91	0.17	1.00	49,49,49,49	0
2	2FL	P	2001	23/23	0.84	0.26	0.99	77,89,100,100	0
3	MG	K	2002	1/1	0.98	0.17	0.95	45,45,45,45	0
3	MG	A	2003	1/1	0.98	0.16	0.93	16,16,16,16	0
4	NA	E	2005	1/1	0.94	0.18	0.82	43,43,43,43	0
4	NA	I	2005	1/1	0.93	0.13	0.66	27,27,27,27	0
4	NA	D	2005	1/1	0.85	0.13	0.59	26,26,26,26	0
4	NA	C	2004	1/1	0.97	0.14	0.56	29,29,29,29	0
4	NA	G	2005	1/1	0.93	0.11	0.48	24,24,24,24	0
4	NA	H	2004	1/1	0.89	0.18	0.47	46,46,46,46	0
4	NA	G	2004	1/1	0.95	0.13	0.36	36,36,36,36	0
3	MG	P	2002	1/1	0.91	0.24	0.29	60,60,60,60	0
2	2FL	I	2001	23/23	0.93	0.16	0.29	49,61,78,100	0
4	NA	H	2005	1/1	0.96	0.13	0.27	33,33,33,33	0
3	MG	I	2003	1/1	0.94	0.14	0.23	26,26,26,26	0
3	MG	J	2003	1/1	0.88	0.14	0.20	24,24,24,24	0
3	MG	M	2003	1/1	0.95	0.23	0.19	41,41,41,41	0
2	2FL	M	2001	23/23	0.88	0.20	0.10	65,77,93,100	0
4	NA	A	2005	1/1	0.81	0.09	0.05	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NA	D	2004	1/1	0.89	0.13	0.03	38,38,38,38	0
4	NA	P	2005	1/1	0.80	0.16	-0.20	55,55,55,55	0
3	MG	O	2003	1/1	0.94	0.14	-0.32	35,35,35,35	0
3	MG	G	2003	1/1	0.88	0.12	-0.33	22,22,22,22	0
4	NA	N	2004	1/1	0.94	0.13	-0.50	44,44,44,44	0
4	NA	F	2004	1/1	0.94	0.12	-0.58	36,36,36,36	0
4	NA	A	2004	1/1	0.92	0.10	-0.82	30,30,30,30	0
3	MG	F	2003	1/1	0.89	0.11	-0.88	22,22,22,22	0
3	MG	K	2003	1/1	0.94	0.13	-1.04	39,39,39,39	0
3	MG	J	2002	1/1	0.97	0.10	-1.06	31,31,31,31	0
3	MG	C	2003	1/1	0.94	0.09	-1.10	15,15,15,15	0
3	MG	M	2002	1/1	0.93	0.15	-1.16	48,48,48,48	0
3	MG	A	2002	1/1	0.98	0.09	-1.20	23,23,23,23	0
4	NA	M	2005	1/1	0.88	0.11	-1.23	43,43,43,43	0
3	MG	E	2003	1/1	0.87	0.14	-1.42	42,42,42,42	0
3	MG	B	2003	1/1	0.94	0.09	-1.59	15,15,15,15	0
4	NA	K	2005	1/1	0.96	0.08	-1.74	40,40,40,40	0
3	MG	L	2003	1/1	0.93	0.11	-1.82	39,39,39,39	0
4	NA	I	2004	1/1	0.97	0.09	-2.06	39,39,39,39	0
3	MG	P	2003	1/1	0.71	0.15	-2.59	53,53,53,53	0
3	MG	N	2003	1/1	0.81	0.09	-2.63	30,30,30,30	0
3	MG	D	2003	1/1	0.94	0.07	-3.01	24,24,24,24	0
4	NA	B	2004	1/1	0.98	0.09	-3.31	29,29,29,29	0
3	MG	H	2003	1/1	0.94	0.09	-3.45	32,32,32,32	0
4	NA	C	2005	1/1	0.92	0.08	-5.51	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.