



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:29 PM UTC

PDB ID : 4V45 / pdb_00004v45
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-F-GALACTOSYL-
ENZYME INTERMEDIATE
Authors : Juers, D.H.; McCarter, J.D.; Withers, S.G.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

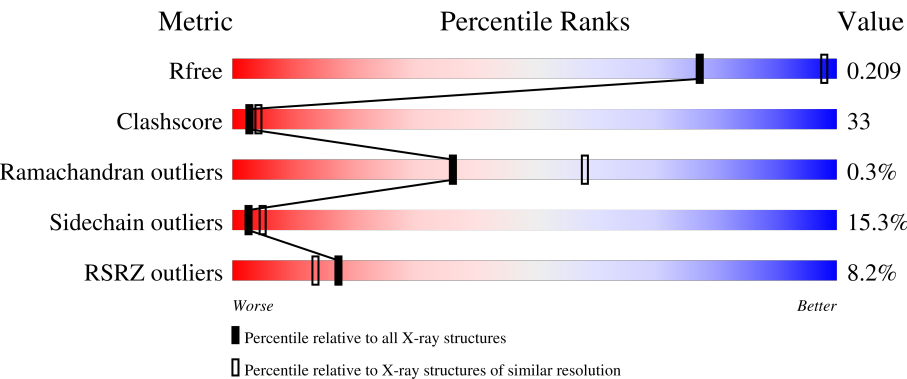
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	1023	5% 43% 42% 13% .
1	B	1023	5% 44% 40% 13% .
1	C	1023	4% 43% 41% 13% .
1	D	1023	6% 43% 41% 13% .
1	E	1023	14% 43% 41% 13% .

Continued on next page...

Continued from previous page...

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	2FG	A	2001	X	-	-	-
2	2FG	B	2001	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FG	C	2001	X	-	-	-
2	2FG	D	2001	X	-	-	-
2	2FG	E	2001	X	-	-	-
2	2FG	F	2001	X	-	-	-
2	2FG	G	2001	X	-	-	-
2	2FG	H	2001	X	-	-	-
2	2FG	I	2001	X	-	-	-
2	2FG	J	2001	X	-	-	-
2	2FG	K	2001	X	-	-	-
2	2FG	L	2001	X	-	-	-
2	2FG	M	2001	X	-	-	-
2	2FG	N	2001	X	-	-	-
2	2FG	O	2001	X	-	-	-
2	2FG	P	2001	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 133984 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:

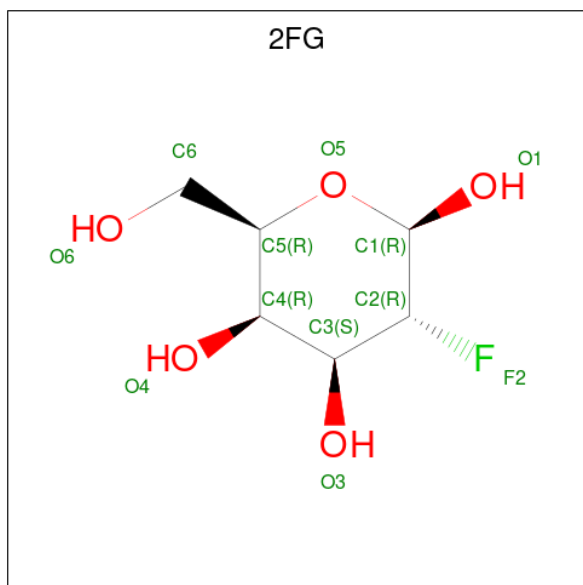
Chain	Residue	Modelled	Actual	Comment	Reference
A	748	CME	CYS	modified residue	UNP P00722
A	914	CME	CYS	modified residue	UNP P00722
A	1021	CME	CYS	modified residue	UNP P00722
B	748	CME	CYS	modified residue	UNP P00722
B	914	CME	CYS	modified residue	UNP P00722
B	1021	CME	CYS	modified residue	UNP P00722
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

Continued on next page...

Continued from previous page...

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 2-deoxy-2-fluoro-beta-D-galactopyranose (CCD ID: 2FG) (formula: $C_6H_{11}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			11	6	1	4		
2	B	1	Total	C	F	O	0	0
			11	6	1	4		
2	C	1	Total	C	F	O	0	0
			11	6	1	4		
2	D	1	Total	C	F	O	0	0
			11	6	1	4		
2	E	1	Total	C	F	O	0	0
			11	6	1	4		
2	F	1	Total	C	F	O	0	0
			11	6	1	4		
2	G	1	Total	C	F	O	0	0
			11	6	1	4		
2	H	1	Total	C	F	O	0	0
			11	6	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	F	O	0	0
			11	6	1	4		
2	J	1	Total	C	F	O	0	0
			11	6	1	4		
2	K	1	Total	C	F	O	0	0
			11	6	1	4		
2	L	1	Total	C	F	O	0	0
			11	6	1	4		
2	M	1	Total	C	F	O	0	0
			11	6	1	4		
2	N	1	Total	C	F	O	0	0
			11	6	1	4		
2	O	1	Total	C	F	O	0	0
			11	6	1	4		
2	P	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	2	Total 2	Na 2	0	0
4	P	2	Total 2	Na 2	0	0

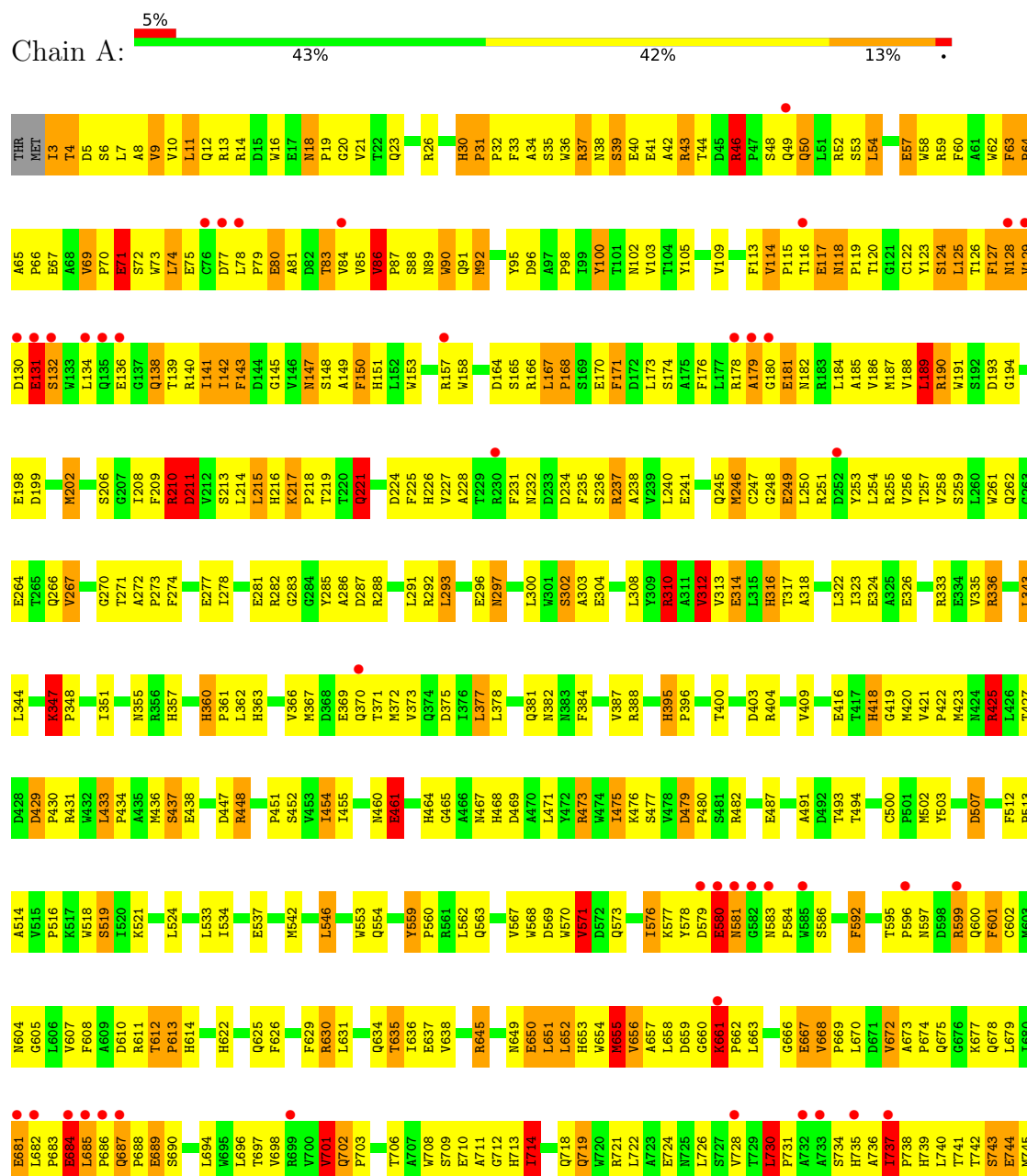
- Molecule 5 is water.

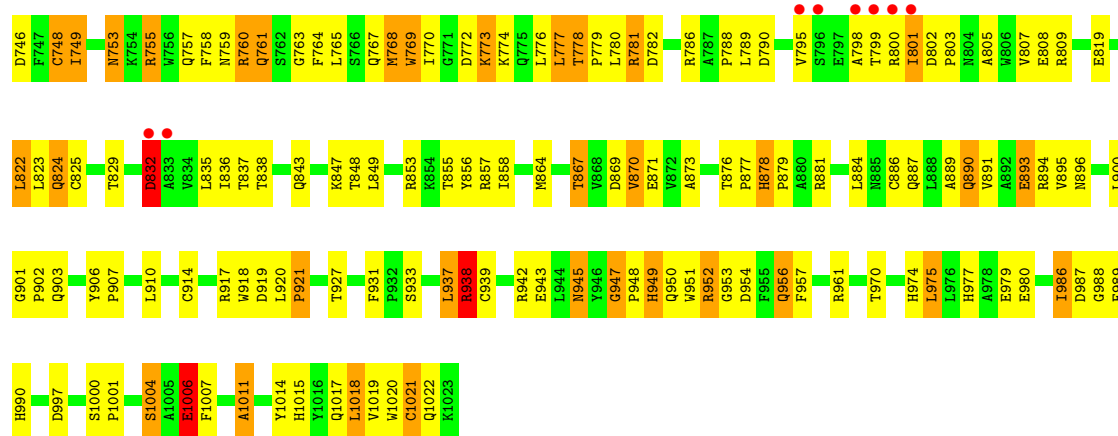
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total 140	O 140	0	0
5	B	140	Total 140	O 140	0	0
5	C	140	Total 140	O 140	0	0
5	D	140	Total 140	O 140	0	0
5	E	139	Total 139	O 139	0	0
5	F	140	Total 140	O 140	0	0
5	G	140	Total 140	O 140	0	0
5	H	141	Total 141	O 141	0	0
5	I	140	Total 140	O 140	0	0
5	J	140	Total 140	O 140	0	0
5	K	140	Total 140	O 140	0	0
5	L	140	Total 140	O 140	0	0
5	M	140	Total 140	O 140	0	0
5	N	140	Total 140	O 140	0	0
5	O	140	Total 140	O 140	0	0
5	P	140	Total 140	O 140	0	0

3 Residue-property plots

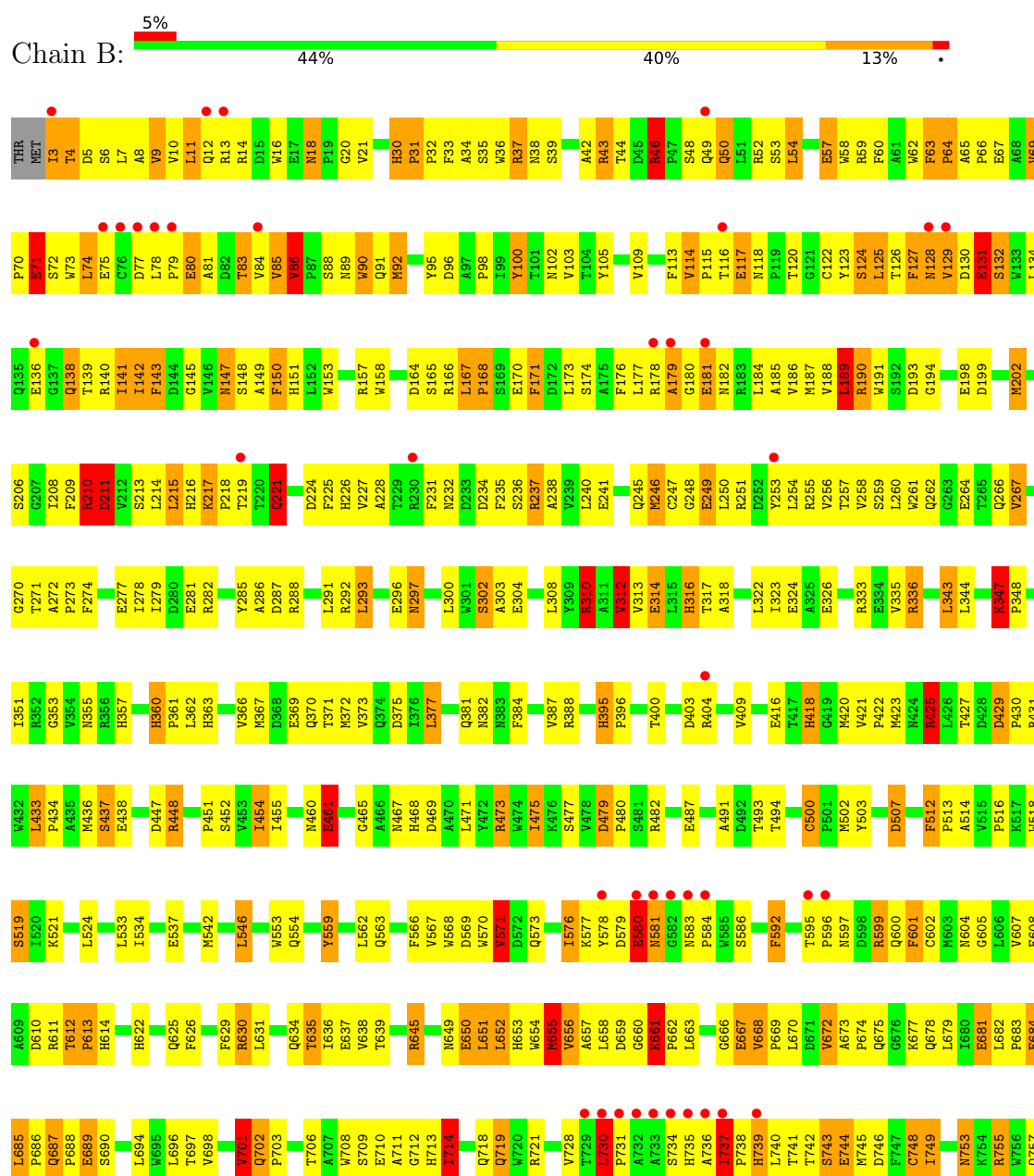
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

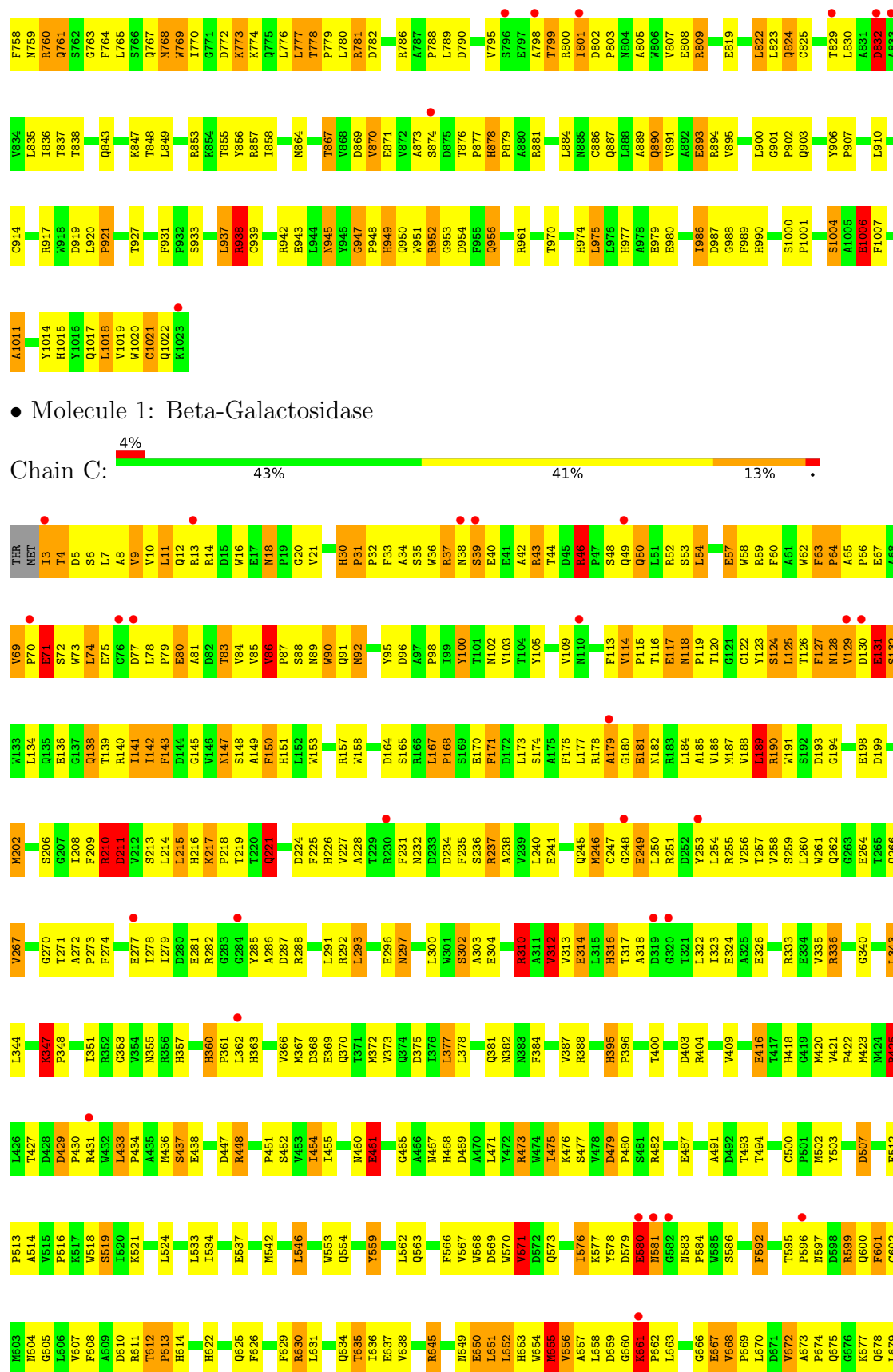
• Molecule 1: Beta-Galactosidase

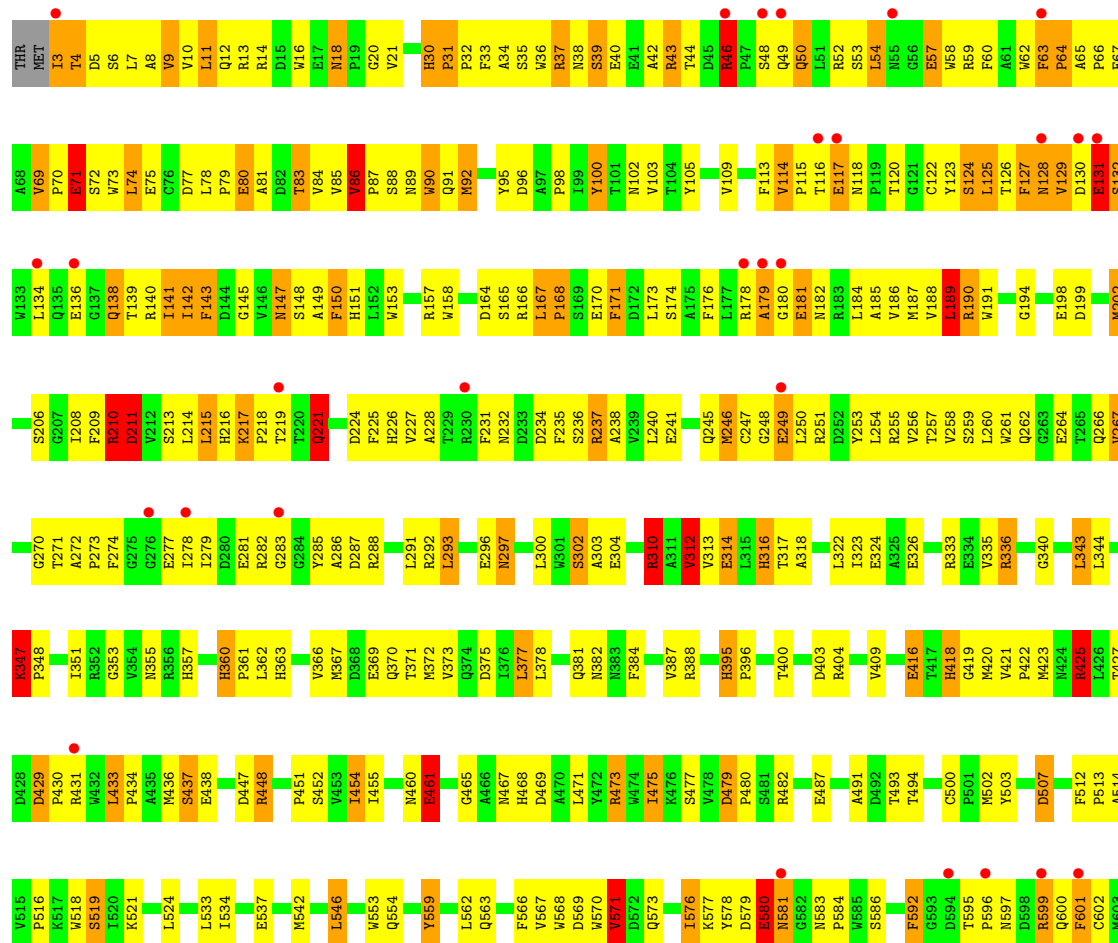


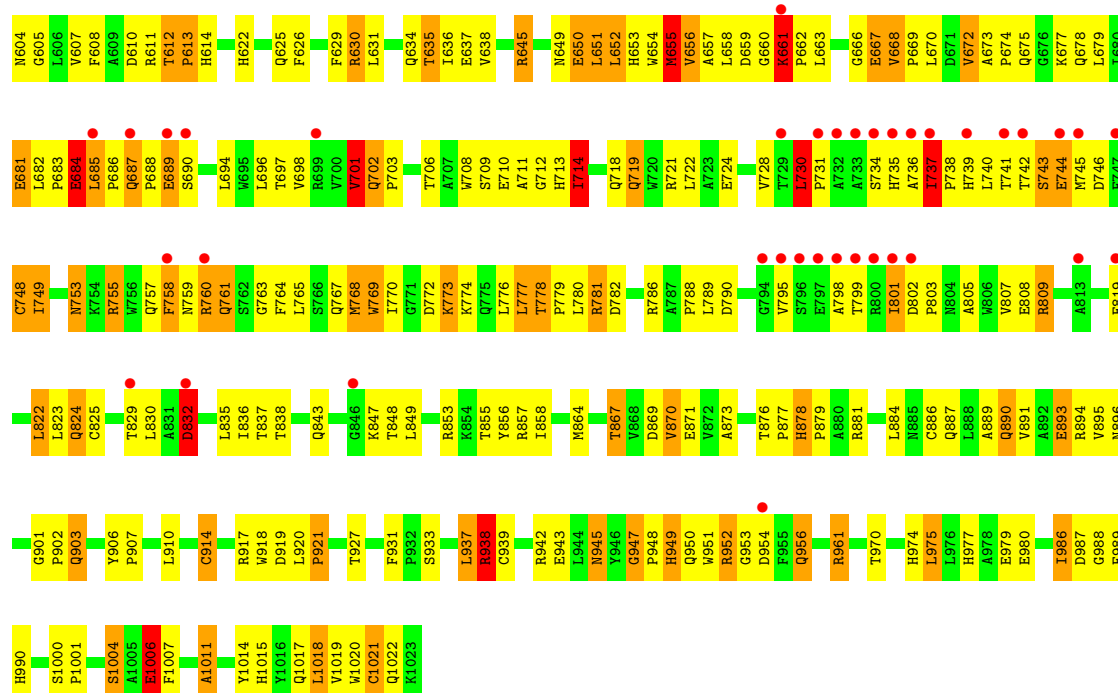


• Molecule 1: Beta-Galactosidase

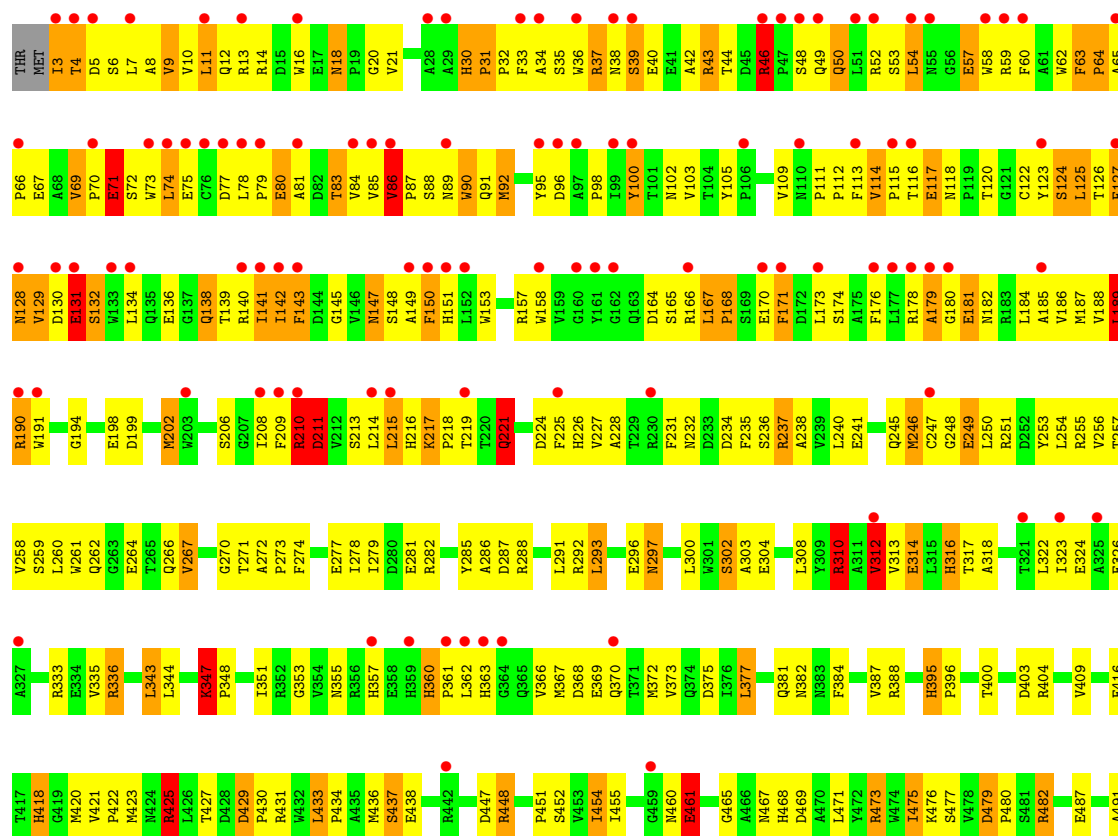
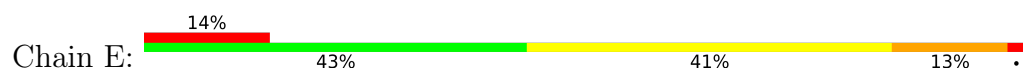


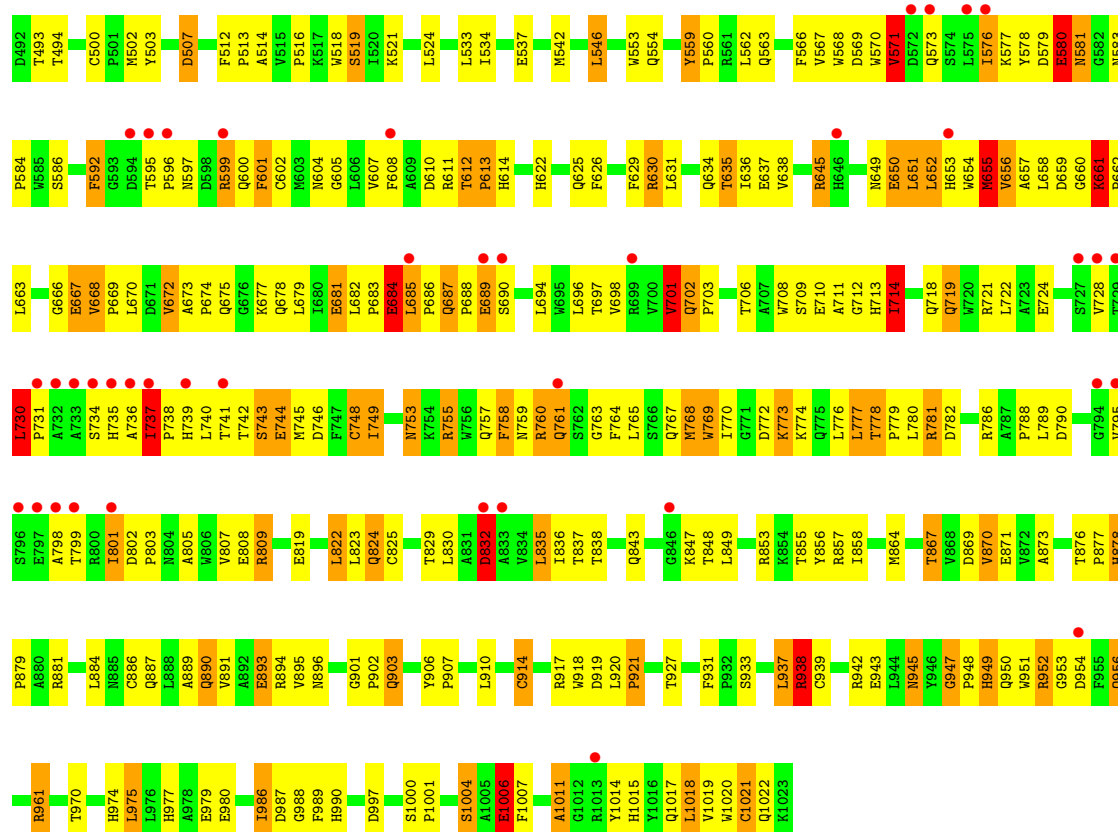




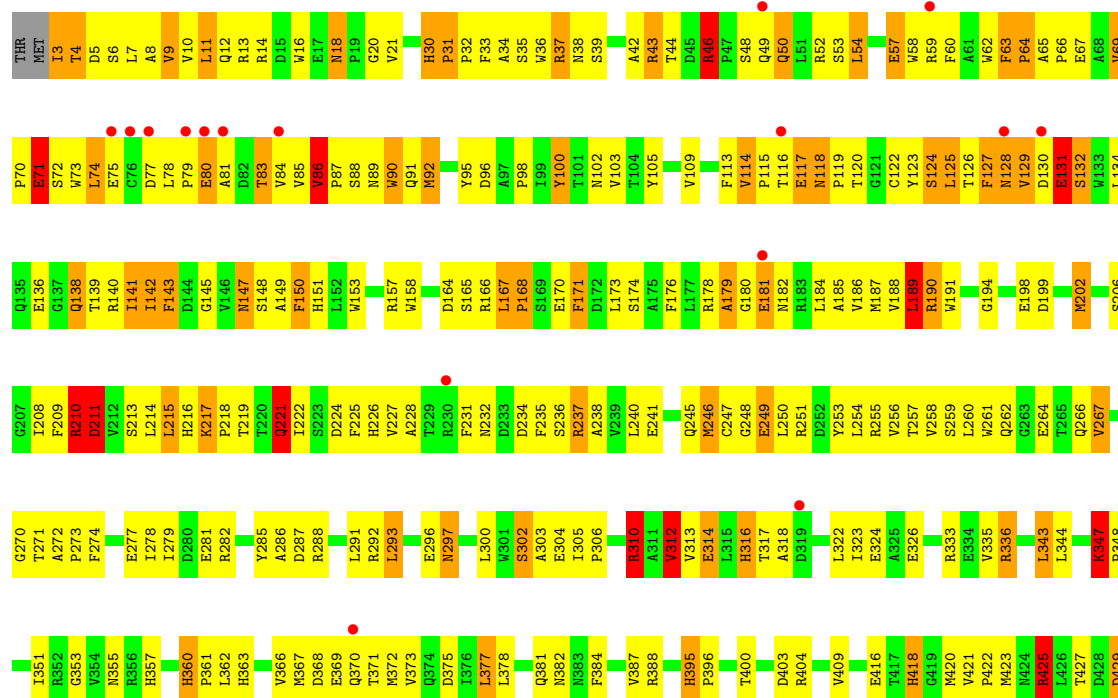
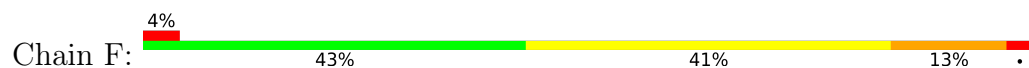


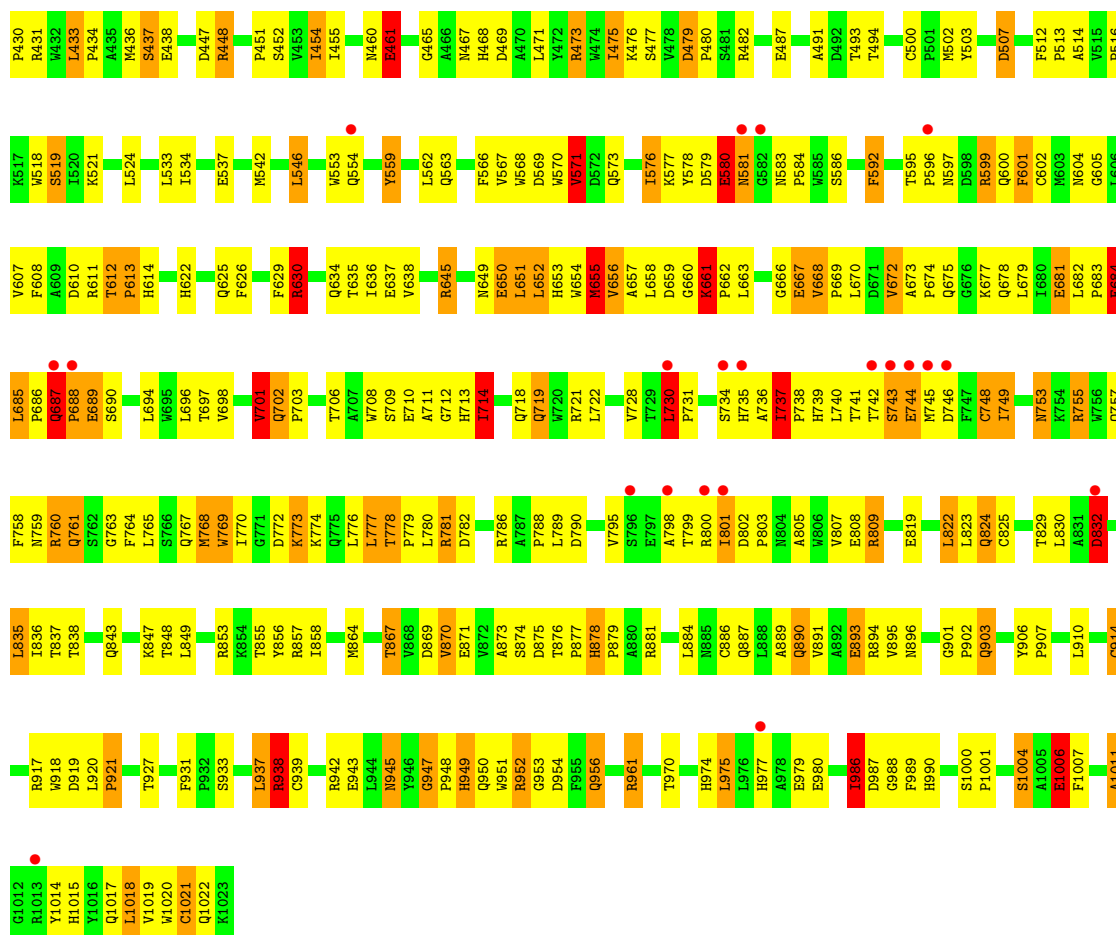
• Molecule 1: Beta-Galactosidase



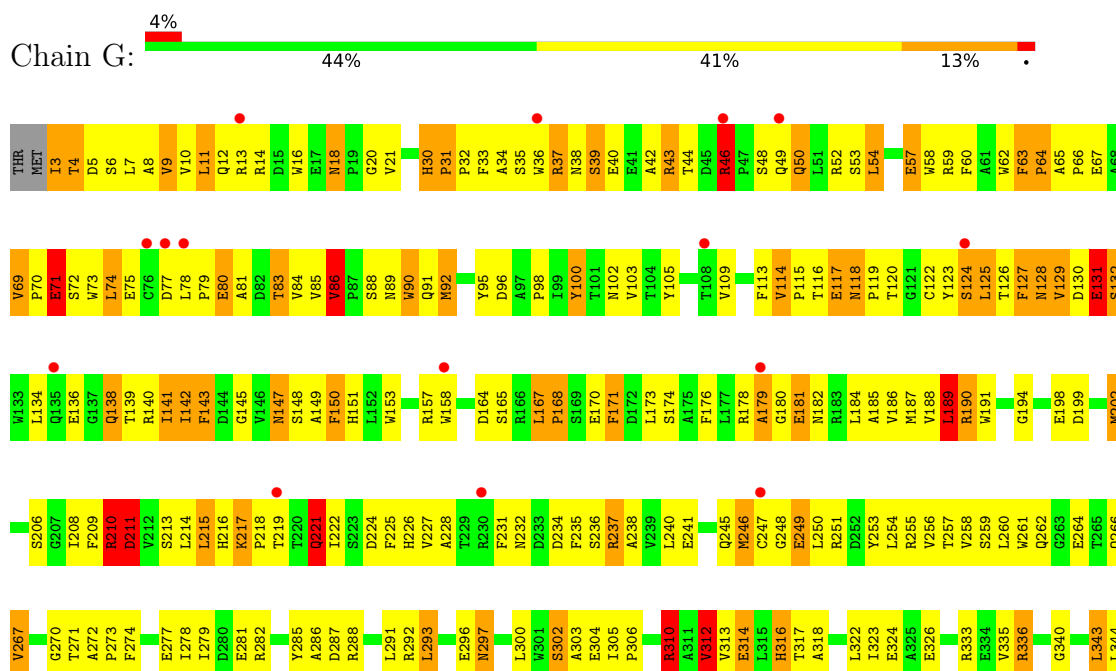


• Molecule 1: Beta-Galactosidase



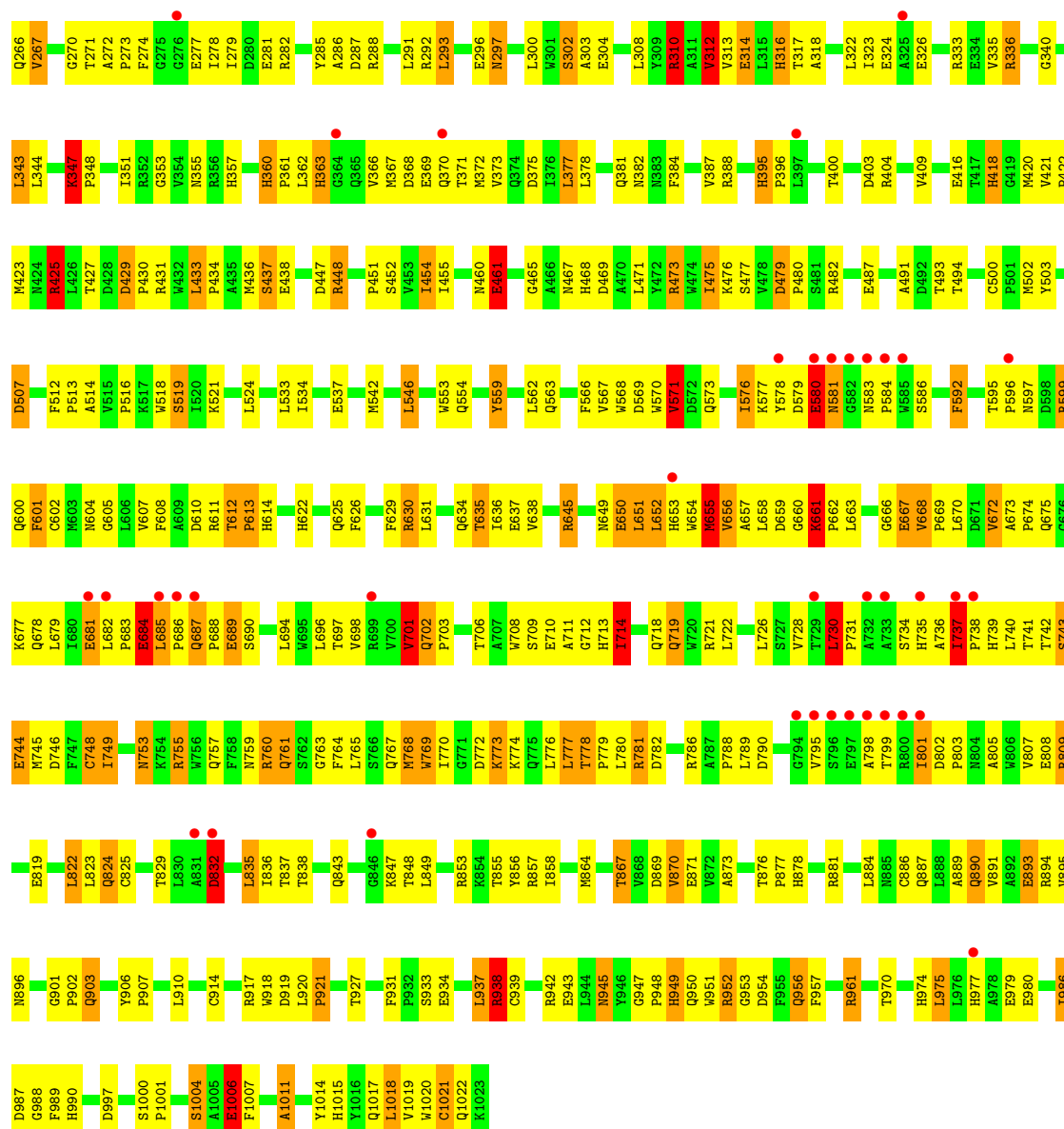


• Molecule 1: Beta-Galactosidase

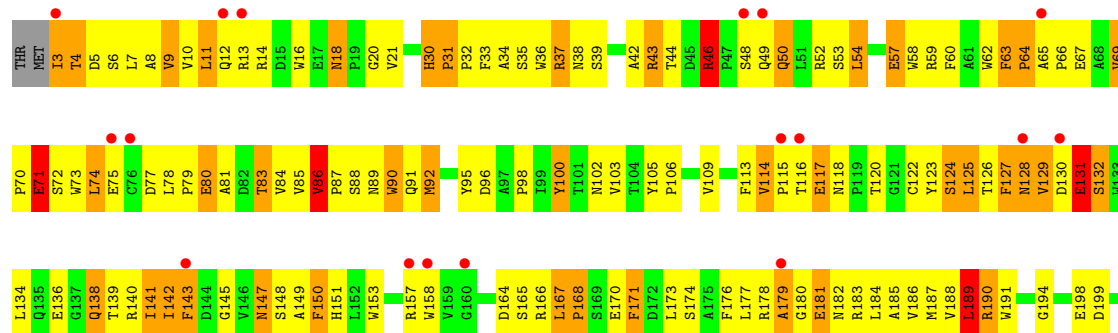


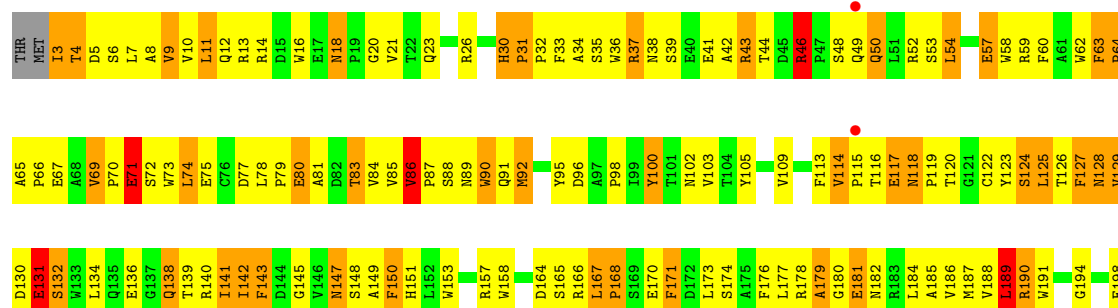


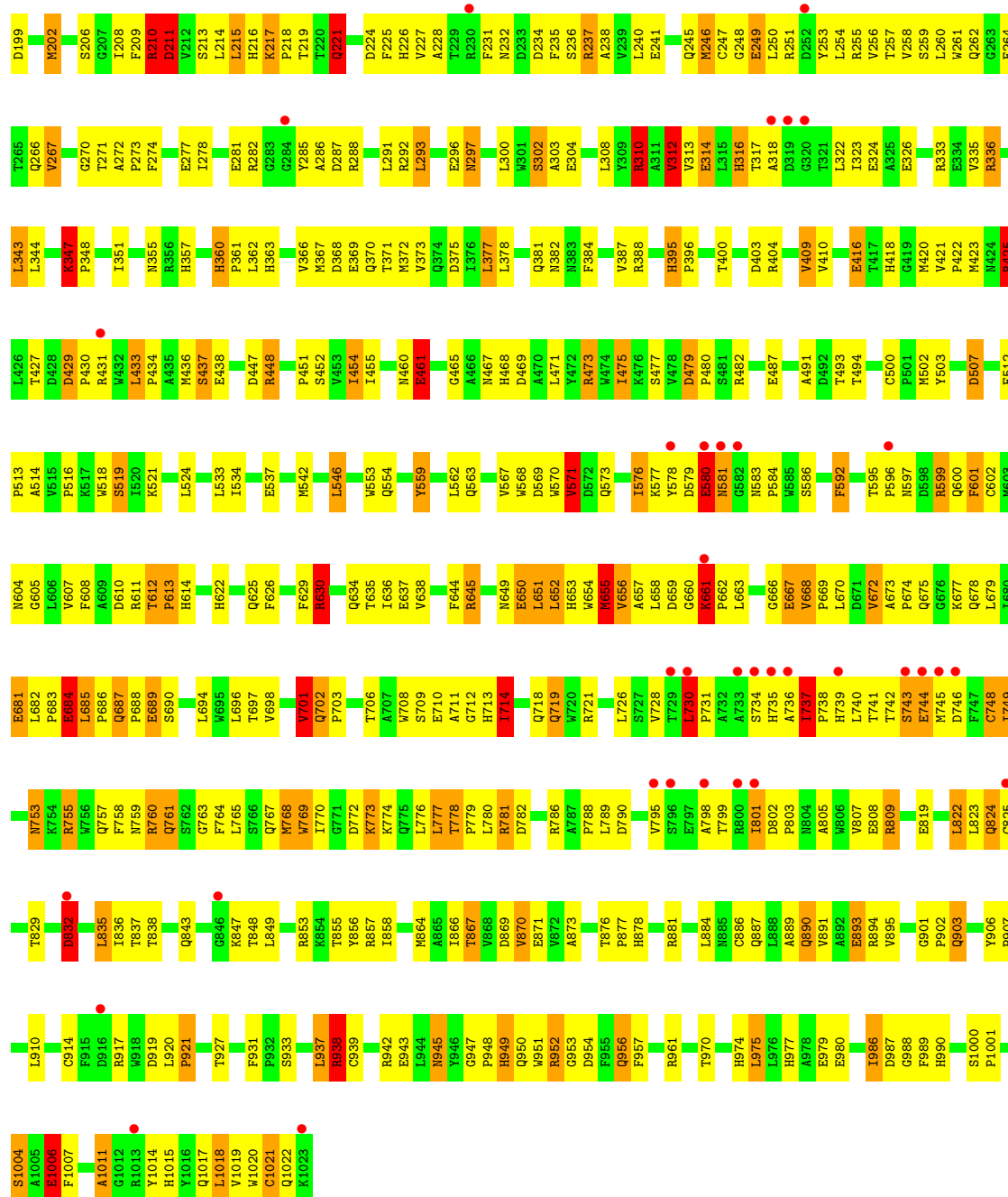
M202	M206	S206	I208	F209	D211	S213	L214	L215	H216	K217	P218	T219	T220	Q221	D224	F225	H226	V227	A228	T229	R230	F231	M232	D233	F234	F235	S236	R237	A238	V239	L240	E241	Q245	M246	C247	G248	E249	R250	R251	D252	V253	L254	R255	V256	T257	V258	S259	L260	W261	Q262	Q263	E264	R265	E266	E267	E268	E269	E270	E271	E272	E273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



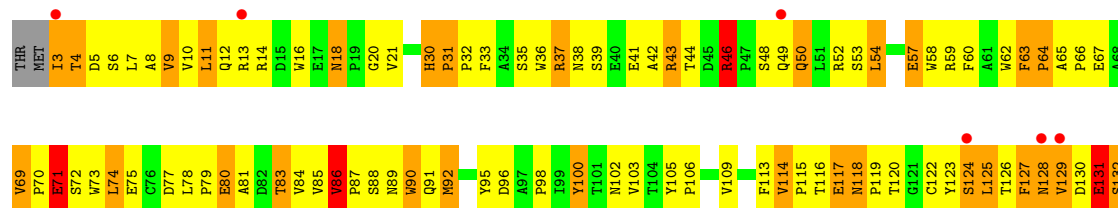
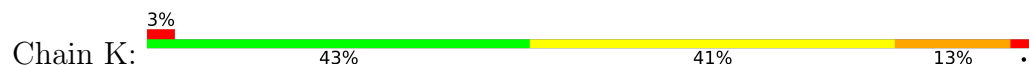
• Molecule 1: Beta-Galactosidase

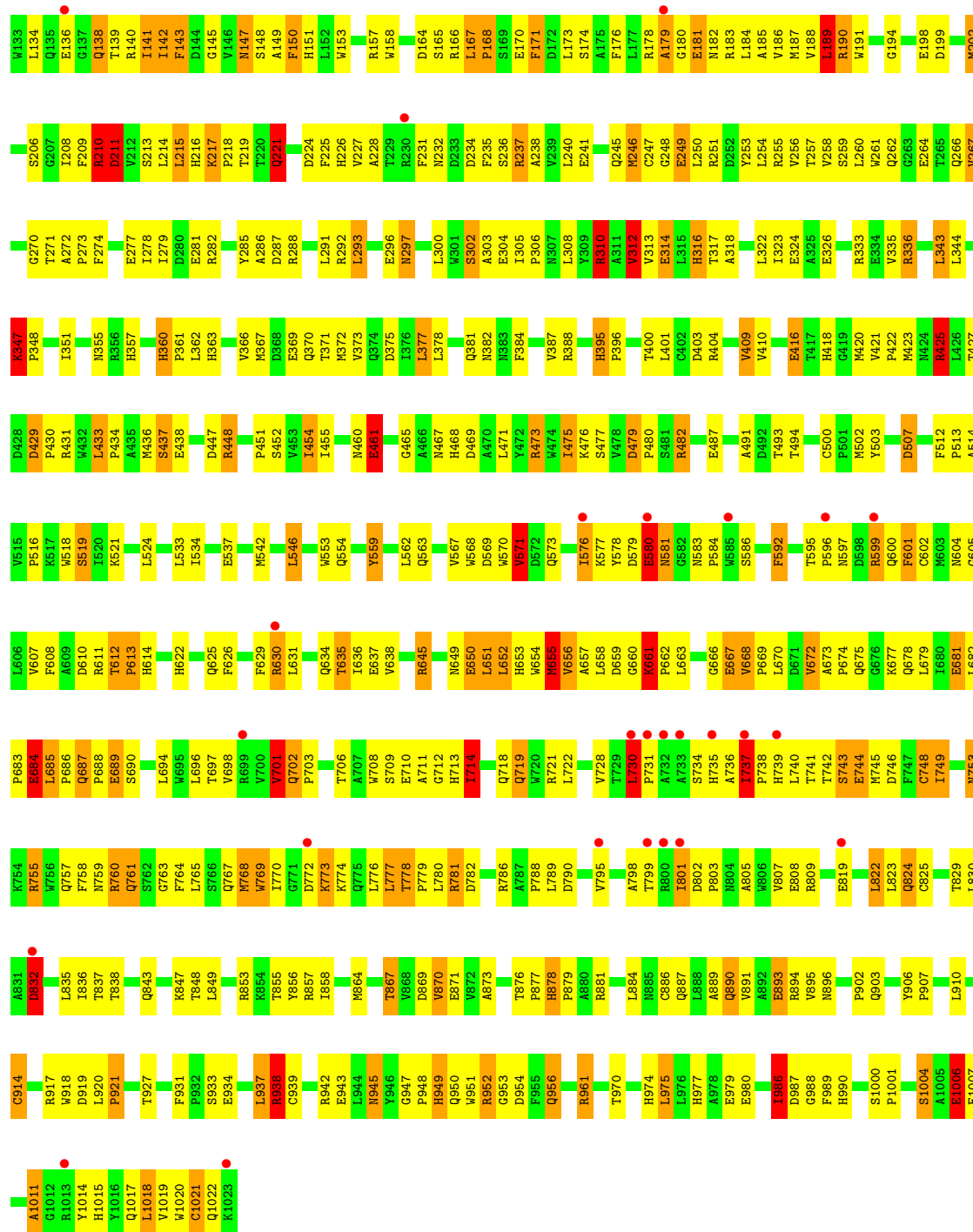




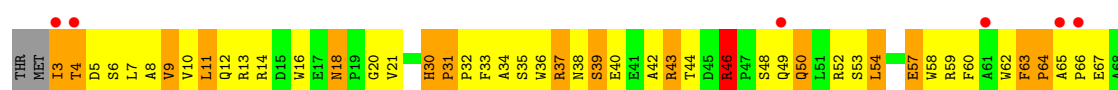


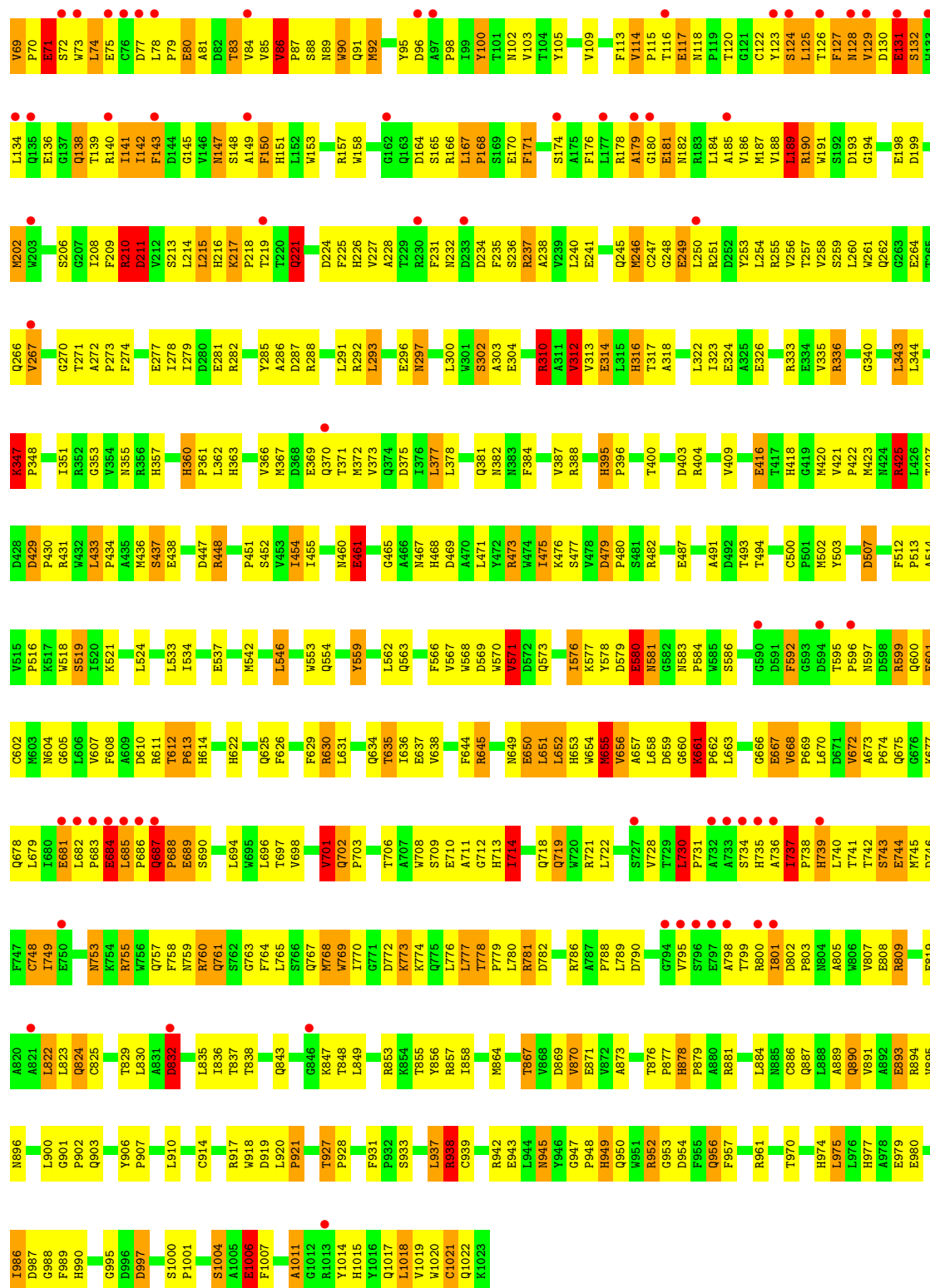
• Molecule 1: Beta-Galactosidase



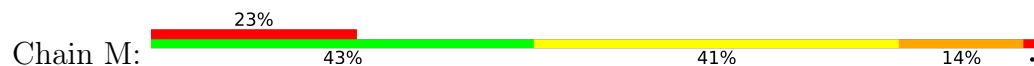


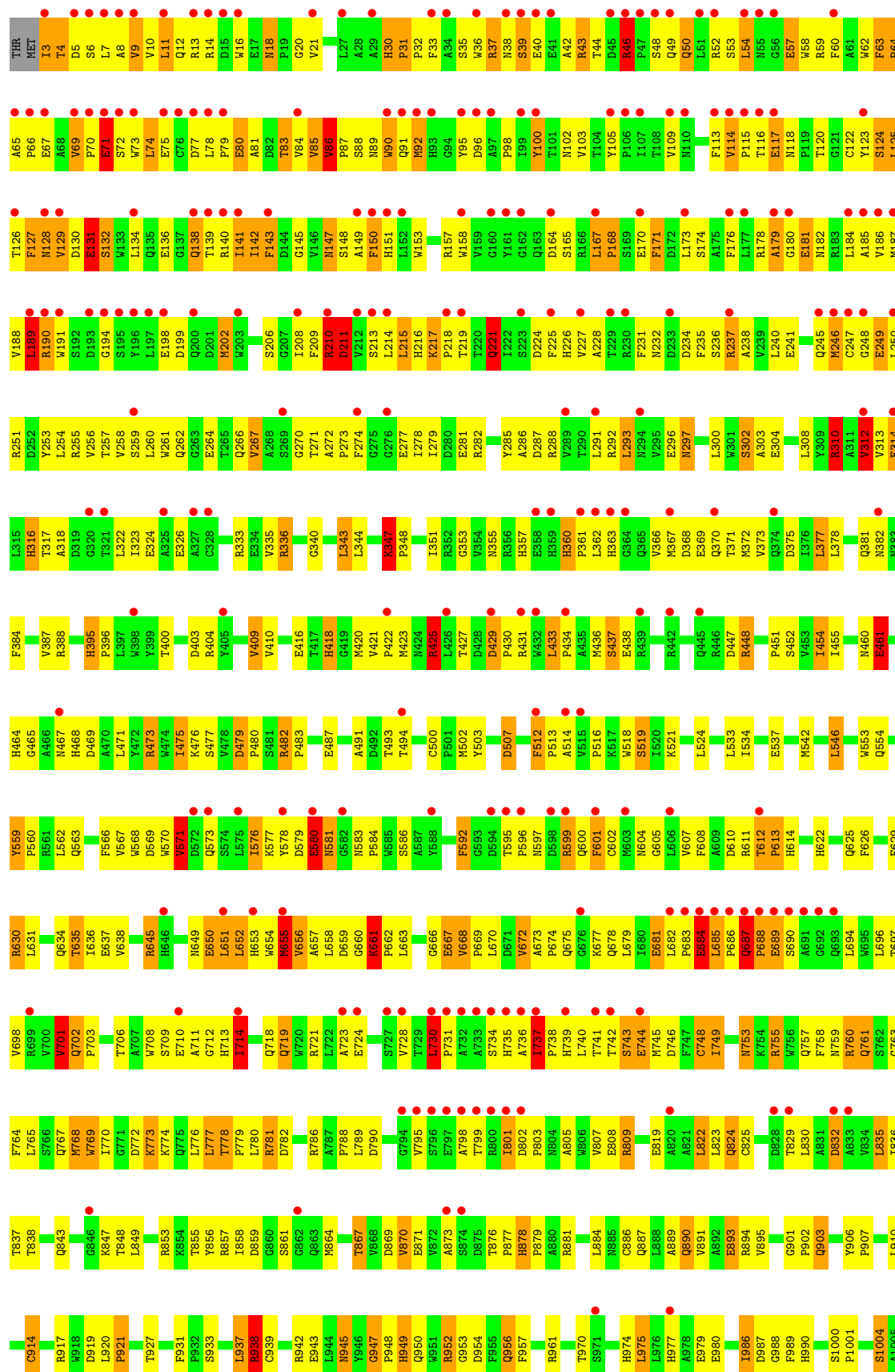
• Molecule 1: Beta-Galactosidase



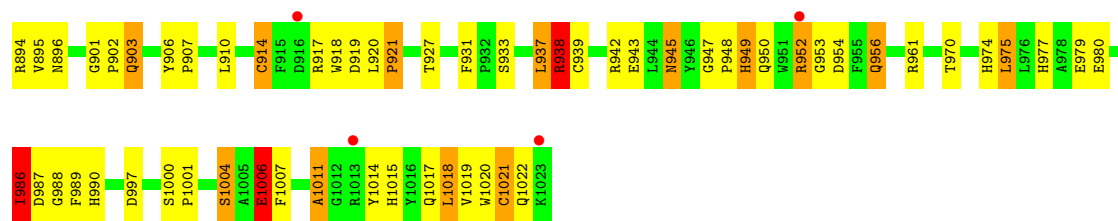


- Molecule 1: Beta-Galactosidase

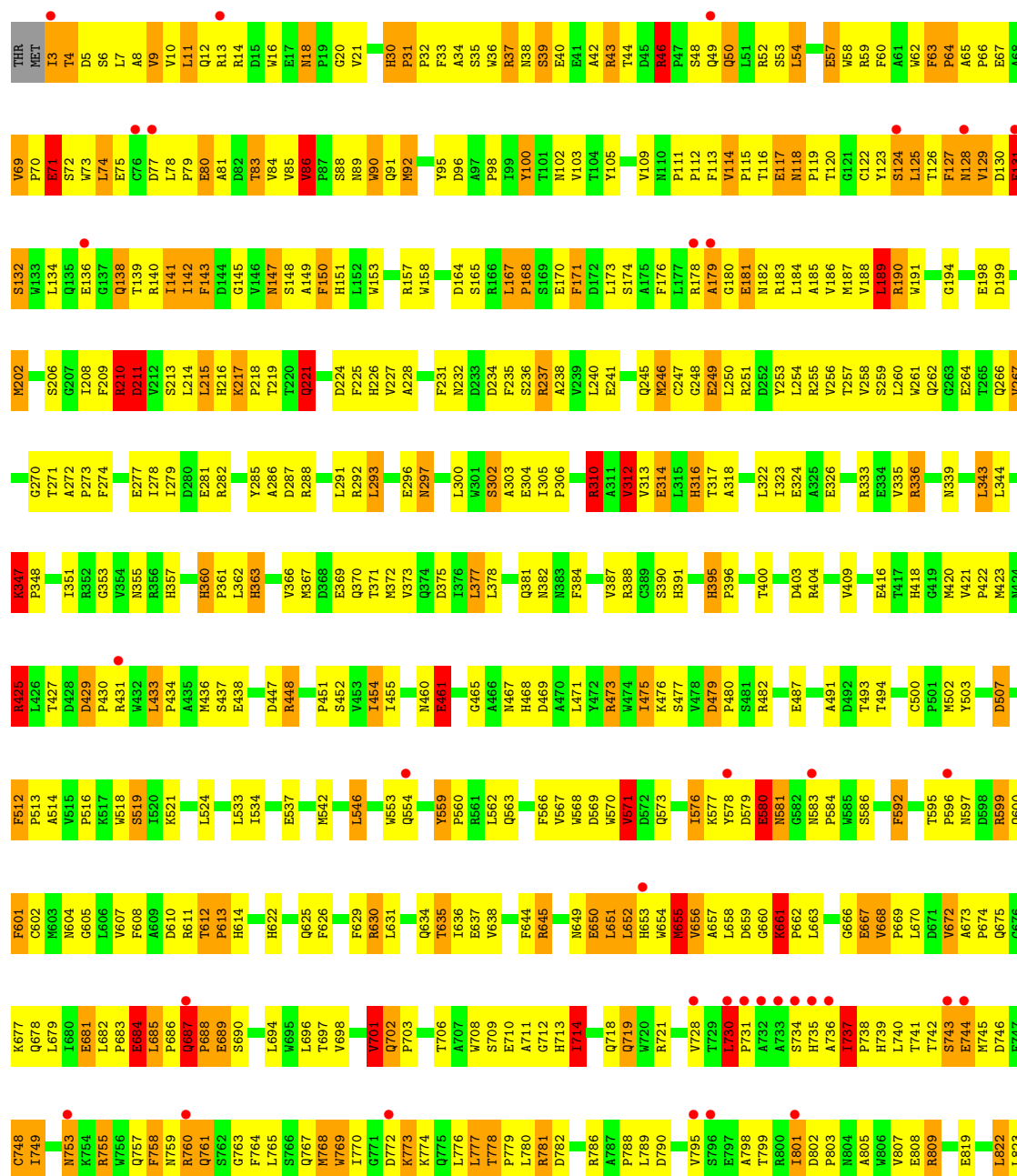
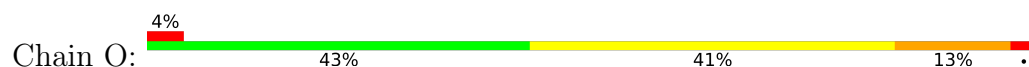


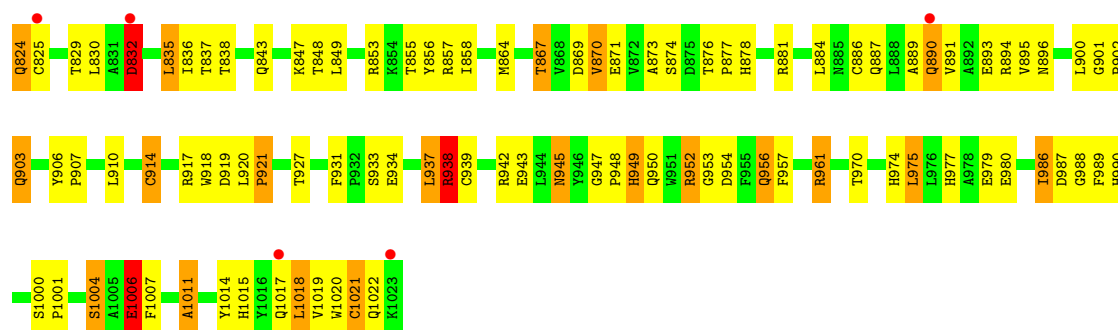


[illegible]

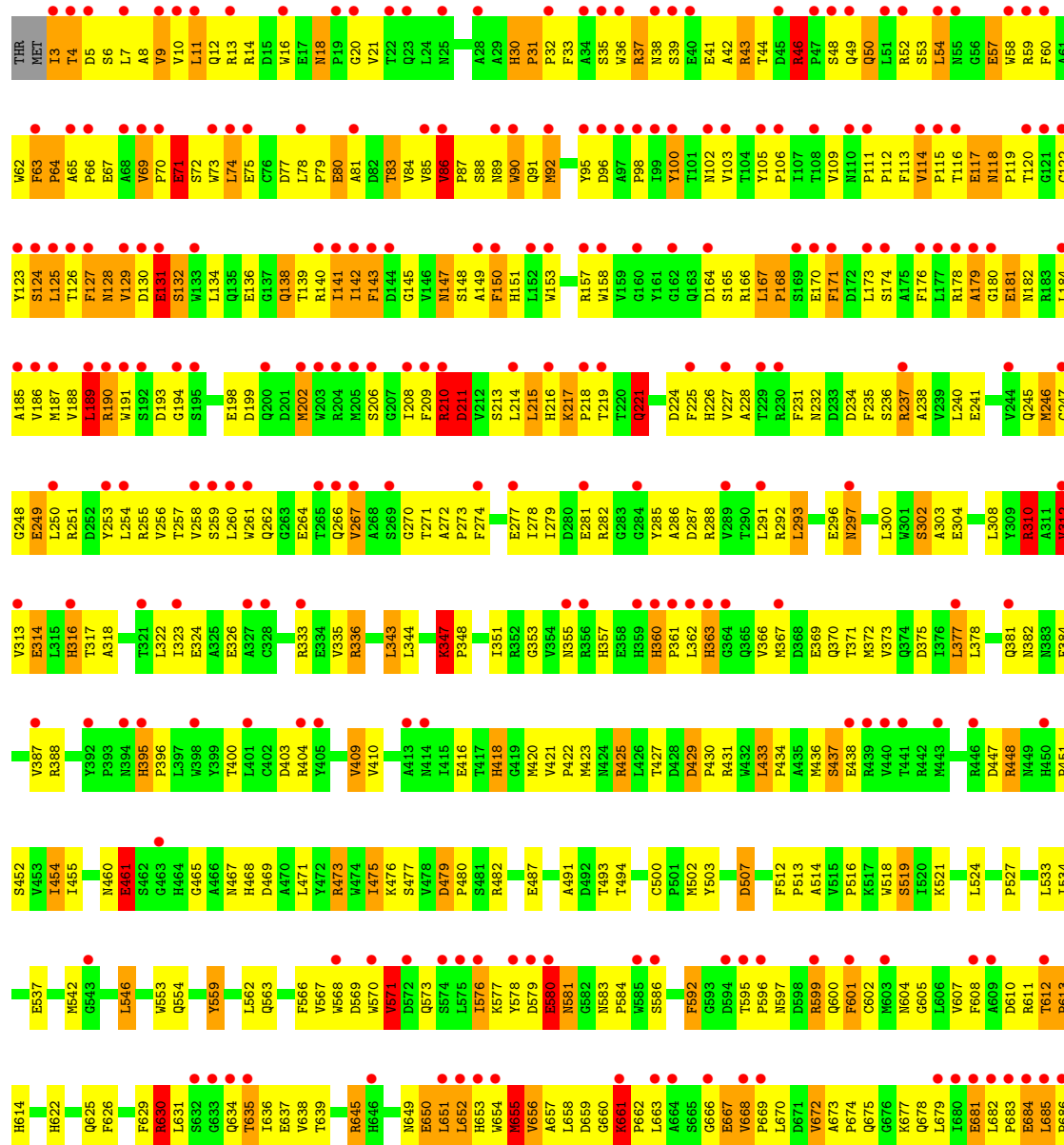
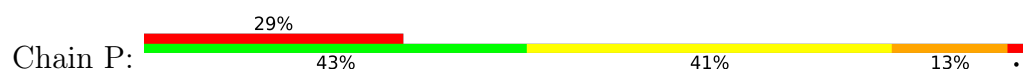


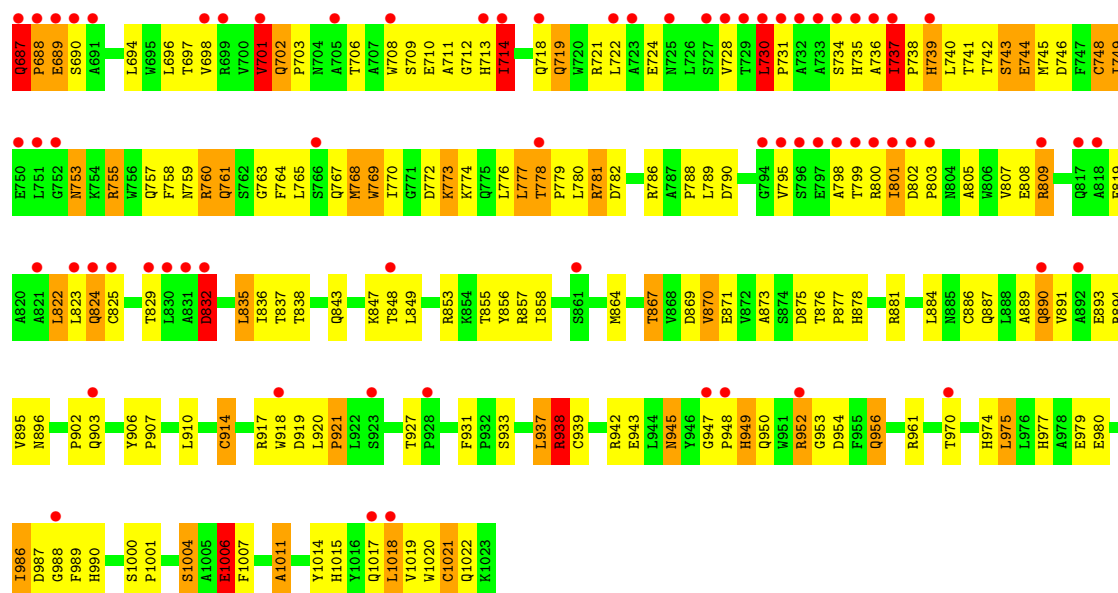
• Molecule 1: Beta-Galactosidase





• Molecule 1: Beta-Galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.50Å 207.20Å 510.20Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	68.50 – 2.60 68.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	70.0 (68.50-2.60) 70.1 (68.50-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.51Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.230 , (Not available) 0.208 , 0.209	Depositor DCC
R_{free} test set	2386 reflections (0.46%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 94.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	133984	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CME, NA, MG, 2FG

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	1.47	33/8439 (0.4%)	1.85	178/11510 (1.5%)
1	B	1.47	34/8439 (0.4%)	1.85	179/11510 (1.6%)
1	C	1.47	32/8439 (0.4%)	1.85	185/11510 (1.6%)
1	D	1.47	34/8439 (0.4%)	1.85	184/11510 (1.6%)
1	E	1.47	33/8439 (0.4%)	1.85	183/11510 (1.6%)
1	F	1.47	32/8439 (0.4%)	1.85	182/11510 (1.6%)
1	G	1.47	32/8439 (0.4%)	1.85	184/11510 (1.6%)
1	H	1.47	33/8439 (0.4%)	1.85	183/11510 (1.6%)
1	I	1.47	32/8439 (0.4%)	1.85	180/11510 (1.6%)
1	J	1.47	32/8439 (0.4%)	1.85	181/11510 (1.6%)
1	K	1.47	32/8439 (0.4%)	1.85	181/11510 (1.6%)
1	L	1.47	32/8439 (0.4%)	1.85	180/11510 (1.6%)
1	M	1.47	32/8439 (0.4%)	1.85	181/11510 (1.6%)
1	N	1.47	32/8439 (0.4%)	1.85	180/11510 (1.6%)
1	O	1.47	30/8439 (0.4%)	1.85	180/11510 (1.6%)
1	P	1.47	32/8439 (0.4%)	1.85	179/11510 (1.6%)
All	All	1.47	517/135024 (0.4%)	1.85	2900/184160 (1.6%)

The worst 5 of 517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	479	ASP	C-N	-7.00	1.26	1.34
1	K	479	ASP	C-N	-6.97	1.26	1.34
1	P	479	ASP	C-N	-6.97	1.26	1.34
1	L	479	ASP	C-N	-6.97	1.26	1.34
1	M	479	ASP	C-N	-6.96	1.26	1.34

The worst 5 of 2900 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	GLY	CA-C-N	-11.56	107.04	123.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	GLY	C-N-CA	-11.56	107.04	123.00
1	D	248	GLY	CA-C-N	-11.56	107.05	123.00
1	D	248	GLY	C-N-CA	-11.56	107.05	123.00
1	H	248	GLY	CA-C-N	-11.55	107.06	123.00

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	8219	0	7812	564	4
1	B	8219	0	7812	526	5
1	C	8219	0	7812	531	2
1	D	8219	0	7812	537	0
1	E	8219	0	7812	528	0
1	F	8219	0	7812	538	0
1	G	8219	0	7812	528	2
1	H	8219	0	7812	549	0
1	I	8219	0	7812	535	2
1	J	8219	0	7812	535	0
1	K	8219	0	7812	529	0
1	L	8219	0	7812	540	2
1	M	8219	0	7812	535	0
1	N	8219	0	7812	536	0
1	O	8219	0	7812	535	1
1	P	8219	0	7812	538	2
2	A	11	0	9	2	0
2	B	11	0	9	2	0
2	C	11	0	9	2	0
2	D	11	0	9	2	0
2	E	11	0	9	2	0
2	F	11	0	9	2	0
2	G	11	0	9	2	0
2	H	11	0	9	2	0
2	I	11	0	9	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	11	0	9	2	0
2	K	11	0	9	2	0
2	L	11	0	9	2	0
2	M	11	0	9	2	0
2	N	11	0	9	2	0
2	O	11	0	9	2	0
2	P	11	0	9	2	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	140	0	0	3	0
5	B	140	0	0	2	0
5	C	140	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	140	0	0	2	0
5	E	139	0	0	2	0
5	F	140	0	0	2	0
5	G	140	0	0	2	0
5	H	141	0	0	2	0
5	I	140	0	0	2	0
5	J	140	0	0	2	0
5	K	140	0	0	2	0
5	L	140	0	0	2	0
5	M	140	0	0	3	0
5	N	140	0	0	2	0
5	O	140	0	0	2	0
5	P	140	0	0	2	0
All	All	133984	0	125136	8466	10

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 33.

The worst 5 of 8466 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:427:THR:HA	1:J:436:MET:HE1	1.15	1.14
1:K:427:THR:HA	1:K:436:MET:HE1	1.15	1.14
1:F:427:THR:HA	1:F:436:MET:HE1	1.15	1.14
1:N:427:THR:HA	1:N:436:MET:HE1	1.15	1.14
1:C:427:THR:HA	1:C:436:MET:HE1	1.15	1.14

The worst 5 of 10 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:G:740:LEU:O	1:L:739:HIS:CD2[1_455]	1.58	0.62
1:B:740:LEU:O	1:P:739:HIS:CD2[1_354]	1.68	0.52
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.72	0.48
1:A:580:GLU:O	1:B:578:TYR:CB[2_555]	1.74	0.46
1:B:739:HIS:NE2	1:P:738:PRO:O[1_354]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	B	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	C	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	36	58
1	D	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	E	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	F	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	G	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	H	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	36	58
1	I	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	J	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	K	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	L	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	M	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	36	58
1	N	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
1	O	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	36	58
1	P	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	36	58
All	All	16288/16368 (100%)	15244 (94%)	996 (6%)	48 (0%)	36	58

5 of 48 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 ⓘ

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%)	738 (85%)	134 (15%)	2	5
1	B	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	C	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	D	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	E	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	F	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	G	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	H	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	I	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	J	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	K	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	L	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	M	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	N	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	O	872/872 (100%)	738 (85%)	134 (15%)	2	5
1	P	872/872 (100%)	738 (85%)	134 (15%)	2	5
All	All	13952/13952 (100%)	11808 (85%)	2144 (15%)	3	5

5 of 2144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	778	THR
1	O	138	GLN
1	N	774	LYS
1	P	477	SER
1	F	773	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 373 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	985	ASN
1	M	316	HIS
1	K	221	GLN
1	L	221	GLN
1	M	1017	GLN

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	P	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	C	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	E	914	1	8,9,10	1.02	0	6,9,11	1.43	1 (16%)
1	CME	A	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	A	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	G	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	H	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)
1	CME	N	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	N	914	1	8,9,10	1.02	0	6,9,11	1.44	1 (16%)
1	CME	O	748	1	8,9,10	0.97	0	6,9,11	1.58	2 (33%)
1	CME	H	914	1	8,9,10	1.03	0	6,9,11	1.44	1 (16%)
1	CME	G	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	I	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)
1	CME	E	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	D	914	1	8,9,10	1.03	0	6,9,11	1.44	1 (16%)
1	CME	D	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	D	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	L	748	1	8,9,10	0.97	0	6,9,11	1.59	2 (33%)
1	CME	I	914	1	8,9,10	1.02	0	6,9,11	1.44	1 (16%)
1	CME	H	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	E	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	F	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	N	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	O	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	B	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	M	914	1	8,9,10	1.02	0	6,9,11	1.44	1 (16%)
1	CME	M	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	F	1021	1	8,9,10	1.10	0	6,9,11	1.45	1 (16%)
1	CME	F	914	1	8,9,10	1.02	0	6,9,11	1.43	1 (16%)
1	CME	B	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)
1	CME	G	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	I	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	O	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	C	748	1	8,9,10	0.97	0	6,9,11	1.59	2 (33%)
1	CME	B	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	J	914	1	8,9,10	1.02	0	6,9,11	1.43	1 (16%)
1	CME	J	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	M	748	1	8,9,10	0.96	0	6,9,11	1.59	2 (33%)
1	CME	P	914	1	8,9,10	1.02	0	6,9,11	1.43	1 (16%)
1	CME	P	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	K	914	1	8,9,10	1.03	0	6,9,11	1.44	1 (16%)
1	CME	K	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)
1	CME	C	1021	1	8,9,10	1.10	0	6,9,11	1.46	1 (16%)
1	CME	J	748	1	8,9,10	0.96	0	6,9,11	1.58	2 (33%)
1	CME	A	748	1	8,9,10	0.97	0	6,9,11	1.59	2 (33%)
1	CME	L	914	1	8,9,10	1.03	0	6,9,11	1.43	1 (16%)
1	CME	L	1021	1	8,9,10	1.09	0	6,9,11	1.46	1 (16%)
1	CME	K	748	1	8,9,10	0.97	0	6,9,11	1.59	2 (33%)

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	P	748	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	E	914	1	-	3/5/8/10	-
1	CME	A	1021	1	-	5/5/8/10	-
1	CME	A	914	1	-	3/5/8/10	-
1	CME	G	1021	1	-	5/5/8/10	-
1	CME	H	1021	1	-	5/5/8/10	-
1	CME	N	748	1	-	3/5/8/10	-
1	CME	N	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	I	1021	1	-	5/5/8/10	-
1	CME	E	748	1	-	3/5/8/10	-
1	CME	D	914	1	-	3/5/8/10	-
1	CME	D	1021	1	-	5/5/8/10	-
1	CME	D	748	1	-	3/5/8/10	-
1	CME	L	748	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	H	748	1	-	3/5/8/10	-
1	CME	E	1021	1	-	5/5/8/10	-
1	CME	F	748	1	-	3/5/8/10	-
1	CME	N	1021	1	-	5/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	B	748	1	-	3/5/8/10	-
1	CME	M	914	1	-	3/5/8/10	-
1	CME	M	1021	1	-	5/5/8/10	-
1	CME	F	1021	1	-	5/5/8/10	-
1	CME	F	914	1	-	3/5/8/10	-
1	CME	B	1021	1	-	5/5/8/10	-
1	CME	G	748	1	-	3/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-
1	CME	O	1021	1	-	5/5/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	C	748	1	-	3/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	J	1021	1	-	5/5/8/10	-
1	CME	M	748	1	-	3/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	P	1021	1	-	5/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-
1	CME	K	1021	1	-	5/5/8/10	-
1	CME	C	1021	1	-	5/5/8/10	-
1	CME	J	748	1	-	3/5/8/10	-
1	CME	A	748	1	-	3/5/8/10	-
1	CME	L	914	1	-	3/5/8/10	-
1	CME	L	1021	1	-	5/5/8/10	-
1	CME	K	748	1	-	3/5/8/10	-

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	914	CME	CB-SG-SD	-2.73	96.80	103.86
1	K	914	CME	CB-SG-SD	-2.72	96.81	103.86
1	I	914	CME	CB-SG-SD	-2.72	96.81	103.86
1	H	914	CME	CB-SG-SD	-2.72	96.81	103.86
1	N	914	CME	CB-SG-SD	-2.72	96.81	103.86

There are no chirality outliers.

5 of 176 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	748	CME	N-CA-CB-SG
1	A	748	CME	SD-CE-CZ-OH
1	A	1021	CME	N-CA-CB-SG
1	A	1021	CME	CE-SD-SG-CB
1	B	748	CME	N-CA-CB-SG

There are no ring outliers.

42 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	748	CME	4	0
1	C	914	CME	1	0
1	E	914	CME	1	0
1	A	1021	CME	6	0
1	G	1021	CME	6	0
1	H	1021	CME	7	0
1	N	748	CME	4	0
1	N	914	CME	1	0
1	O	748	CME	4	0
1	G	914	CME	1	0
1	I	1021	CME	6	0
1	E	748	CME	4	0
1	D	914	CME	1	0
1	D	1021	CME	6	0
1	D	748	CME	4	0
1	L	748	CME	4	0
1	H	748	CME	4	0
1	E	1021	CME	6	0
1	F	748	CME	4	0
1	N	1021	CME	6	0
1	O	914	CME	1	0
1	B	748	CME	4	0
1	M	914	CME	1	0
1	M	1021	CME	6	0
1	F	1021	CME	6	0
1	F	914	CME	1	0
1	B	1021	CME	6	0
1	G	748	CME	4	0
1	I	748	CME	4	0
1	O	1021	CME	7	0
1	C	748	CME	4	0
1	J	1021	CME	6	0
1	M	748	CME	4	0
1	P	914	CME	1	0
1	P	1021	CME	6	0
1	K	914	CME	1	0
1	K	1021	CME	6	0
1	C	1021	CME	7	0
1	J	748	CME	4	0
1	A	748	CME	4	0
1	L	1021	CME	6	0
1	K	748	CME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	2FG	J	2001	1,4	11,11,12	1.25	1 (9%)	12,15,17	1.48	3 (25%)
2	2FG	L	2001	1,4	11,11,12	1.25	0	12,15,17	1.48	3 (25%)
2	2FG	M	2001	1,4	11,11,12	1.25	1 (9%)	12,15,17	1.48	3 (25%)
2	2FG	D	2001	1,4	11,11,12	1.25	0	12,15,17	1.49	3 (25%)
2	2FG	A	2001	1,4	11,11,12	1.25	0	12,15,17	1.48	3 (25%)
2	2FG	F	2001	1,4	11,11,12	1.26	0	12,15,17	1.48	3 (25%)
2	2FG	O	2001	1,4	11,11,12	1.24	0	12,15,17	1.47	3 (25%)
2	2FG	B	2001	1,4	11,11,12	1.25	0	12,15,17	1.48	3 (25%)
2	2FG	H	2001	1,4	11,11,12	1.24	0	12,15,17	1.48	3 (25%)
2	2FG	K	2001	1,4	11,11,12	1.24	0	12,15,17	1.48	3 (25%)
2	2FG	P	2001	1,4	11,11,12	1.25	0	12,15,17	1.48	3 (25%)
2	2FG	E	2001	1,4	11,11,12	1.25	1 (9%)	12,15,17	1.48	3 (25%)
2	2FG	I	2001	1,4	11,11,12	1.25	0	12,15,17	1.48	3 (25%)
2	2FG	G	2001	1,4	11,11,12	1.23	0	12,15,17	1.49	3 (25%)
2	2FG	N	2001	1,4	11,11,12	1.24	1 (9%)	12,15,17	1.48	3 (25%)
2	2FG	C	2001	1,4	11,11,12	1.24	0	12,15,17	1.49	3 (25%)

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	2FG	J	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	L	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	M	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	D	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	A	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	F	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	O	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	B	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	H	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	K	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	P	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	E	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	I	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	G	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	N	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	C	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2001	2FG	C4-C5	2.02	1.57	1.53
2	N	2001	2FG	C4-C5	2.02	1.57	1.53
2	J	2001	2FG	C4-C5	2.01	1.57	1.53
2	M	2001	2FG	C4-C5	2.00	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	2FG	O5-C5-C6	-3.26	101.32	107.66
2	N	2001	2FG	O5-C5-C6	-3.26	101.32	107.66
2	G	2001	2FG	O5-C5-C6	-3.26	101.32	107.66
2	B	2001	2FG	O5-C5-C6	-3.25	101.33	107.66
2	A	2001	2FG	O5-C5-C6	-3.25	101.33	107.66

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	2FG	C1
2	B	2001	2FG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	C	2001	2FG	C1
2	D	2001	2FG	C1
2	E	2001	2FG	C1

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	2FG	O5-C5-C6-O6
2	H	2001	2FG	O5-C5-C6-O6
2	I	2001	2FG	O5-C5-C6-O6
2	L	2001	2FG	O5-C5-C6-O6
2	M	2001	2FG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2001	2FG	2	0
2	L	2001	2FG	2	0
2	M	2001	2FG	2	0
2	D	2001	2FG	2	0
2	A	2001	2FG	2	0
2	F	2001	2FG	2	0
2	O	2001	2FG	2	0
2	B	2001	2FG	2	0
2	H	2001	2FG	2	0
2	K	2001	2FG	2	0
2	P	2001	2FG	2	0
2	E	2001	2FG	2	0
2	I	2001	2FG	2	0
2	G	2001	2FG	2	0
2	N	2001	2FG	2	0
2	C	2001	2FG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	1018/1023 (99%)	0.14	50 (4%) 35 29	9, 32, 74, 100	5 (0%)
1	B	1018/1023 (99%)	0.13	47 (4%) 37 32	7, 31, 72, 99	5 (0%)
1	C	1018/1023 (99%)	0.14	46 (4%) 38 32	6, 29, 70, 97	5 (0%)
1	D	1018/1023 (99%)	0.41	65 (6%) 25 20	11, 35, 76, 100	5 (0%)
1	E	1018/1023 (99%)	0.97	145 (14%) 6 5	23, 47, 84, 100	5 (0%)
1	F	1018/1023 (99%)	0.10	37 (3%) 46 40	9, 33, 74, 100	5 (0%)
1	G	1018/1023 (99%)	0.26	46 (4%) 38 32	13, 37, 77, 100	5 (0%)
1	H	1018/1023 (99%)	0.71	92 (9%) 15 11	21, 45, 82, 100	5 (0%)
1	I	1018/1023 (99%)	0.36	44 (4%) 40 34	17, 40, 80, 100	5 (0%)
1	J	1018/1023 (99%)	0.19	37 (3%) 46 40	15, 38, 78, 100	5 (0%)
1	K	1018/1023 (99%)	0.41	32 (3%) 51 45	25, 49, 85, 100	5 (0%)
1	L	1018/1023 (99%)	0.64	70 (6%) 23 18	24, 48, 85, 100	5 (0%)
1	M	1018/1023 (99%)	1.32	238 (23%) 2 1	27, 51, 86, 100	5 (0%)
1	N	1018/1023 (99%)	0.30	45 (4%) 39 33	17, 40, 80, 100	5 (0%)
1	O	1018/1023 (99%)	0.27	39 (3%) 44 38	17, 41, 80, 100	5 (0%)
1	P	1018/1023 (99%)	1.61	299 (29%) 1 1	32, 55, 90, 100	5 (0%)
All	All	16288/16368 (99%)	0.50	1332 (8%) 17 14	6, 42, 80, 100	80 (0%)

The worst 5 of 1332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.5
1	B	582	GLY	6.4
1	A	682	LEU	6.3
1	P	739	HIS	6.2
1	A	581	ASN	6.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
1	CME	P	914	10/11	0.80	0.20	42,47,100,100	0
1	CME	L	748	10/11	0.83	0.16	43,63,100,100	0
1	CME	P	1021	10/11	0.83	0.18	53,74,100,100	0
1	CME	O	748	10/11	0.86	0.23	36,56,98,100	0
1	CME	B	748	10/11	0.87	0.17	25,46,87,98	0
1	CME	D	748	10/11	0.87	0.17	29,50,92,100	0
1	CME	E	748	10/11	0.87	0.17	41,61,100,100	0
1	CME	K	1021	10/11	0.87	0.13	46,67,100,100	0
1	CME	N	1021	10/11	0.88	0.15	38,59,100,100	0
1	CME	K	748	10/11	0.88	0.14	43,64,100,100	0
1	CME	P	748	10/11	0.88	0.16	50,70,100,100	0
1	CME	I	748	10/11	0.88	0.18	35,55,97,100	0
1	CME	J	1021	10/11	0.88	0.17	36,57,100,100	0
1	CME	I	1021	10/11	0.89	0.16	38,59,100,100	0
1	CME	C	748	10/11	0.89	0.15	23,44,86,96	0
1	CME	O	1021	10/11	0.89	0.15	39,60,100,100	0
1	CME	E	1021	10/11	0.89	0.15	44,65,100,100	0
1	CME	H	1021	10/11	0.89	0.15	42,63,100,100	0
1	CME	D	1021	10/11	0.89	0.18	32,54,100,100	0
1	CME	F	1021	10/11	0.90	0.13	30,51,100,100	0
1	CME	C	1021	10/11	0.90	0.14	26,48,96,96	0
1	CME	M	748	10/11	0.91	0.16	45,65,100,100	0
1	CME	M	1021	10/11	0.91	0.15	48,69,100,100	0
1	CME	A	1021	10/11	0.91	0.12	30,51,100,100	0
1	CME	J	748	10/11	0.91	0.15	33,53,95,100	0
1	CME	G	1021	10/11	0.91	0.14	34,55,100,100	0
1	CME	H	748	10/11	0.91	0.14	39,59,100,100	0
1	CME	B	1021	10/11	0.91	0.15	28,49,98,98	0
1	CME	F	748	10/11	0.91	0.14	27,47,89,100	0
1	CME	L	1021	10/11	0.92	0.12	46,67,100,100	0
1	CME	K	914	10/11	0.92	0.13	36,40,99,100	0
1	CME	M	914	10/11	0.92	0.15	38,42,100,100	0
1	CME	G	748	10/11	0.92	0.14	31,51,93,100	0
1	CME	H	914	10/11	0.92	0.14	32,36,95,100	0
1	CME	N	748	10/11	0.93	0.13	35,55,97,100	0
1	CME	A	748	10/11	0.93	0.12	27,47,89,100	0
1	CME	L	914	10/11	0.93	0.12	35,40,99,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	O	914	10/11	0.93	0.12	28,33,92,100	0
1	CME	E	914	10/11	0.95	0.12	34,38,97,100	0
1	CME	N	914	10/11	0.95	0.12	27,32,91,100	0
1	CME	J	914	10/11	0.95	0.13	25,30,89,100	0
1	CME	A	914	10/11	0.96	0.10	19,24,83,96	0
1	CME	B	914	10/11	0.96	0.10	18,22,82,95	0
1	CME	I	914	10/11	0.96	0.11	27,32,91,100	0
1	CME	F	914	10/11	0.96	0.10	20,24,83,97	0
1	CME	D	914	10/11	0.96	0.12	22,27,86,99	0
1	CME	C	914	10/11	0.97	0.10	16,21,80,93	0
1	CME	G	914	10/11	0.97	0.09	24,28,87,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	2FG	P	2001	11/12	0.66	0.20	48,52,58,63	0
4	NA	O	2005	1/1	0.70	0.12	37,37,37,37	0
2	2FG	M	2001	11/12	0.73	0.17	43,47,54,58	0
2	2FG	H	2001	11/12	0.75	0.15	37,41,48,52	0
4	NA	M	2004	1/1	0.77	0.19	62,62,62,62	0
2	2FG	E	2001	11/12	0.77	0.12	39,43,49,54	0
2	2FG	L	2001	11/12	0.80	0.15	41,45,51,56	0
4	NA	L	2004	1/1	0.81	0.14	60,60,60,60	0
4	NA	G	2005	1/1	0.82	0.10	32,32,32,32	0
4	NA	P	2004	1/1	0.82	0.13	67,67,67,67	0
3	MG	P	2002	1/1	0.83	0.16	47,47,47,47	0
2	2FG	I	2001	11/12	0.83	0.12	33,37,43,48	0
4	NA	D	2005	1/1	0.86	0.09	31,31,31,31	0
3	MG	I	2002	1/1	0.86	0.11	32,32,32,32	0
4	NA	J	2004	1/1	0.87	0.26	50,50,50,50	0
4	NA	K	2005	1/1	0.88	0.10	44,44,44,44	0
3	MG	L	2002	1/1	0.89	0.13	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	I	2005	1/1	0.90	0.09	36,36,36,36	0
3	MG	M	2002	1/1	0.90	0.11	43,43,43,43	0
4	NA	M	2005	1/1	0.90	0.17	46,46,46,46	0
4	NA	J	2005	1/1	0.90	0.07	34,34,34,34	0
3	MG	D	2003	1/1	0.90	0.13	27,27,27,27	0
4	NA	I	2004	1/1	0.91	0.10	52,52,52,52	0
3	MG	O	2003	1/1	0.91	0.13	33,33,33,33	0
2	2FG	F	2001	11/12	0.91	0.12	25,29,36,40	0
4	NA	N	2005	1/1	0.91	0.11	36,36,36,36	0
2	2FG	J	2001	11/12	0.91	0.13	31,35,41,46	0
2	2FG	A	2001	11/12	0.91	0.10	25,29,35,40	0
4	NA	B	2004	1/1	0.92	0.09	42,42,42,42	0
4	NA	B	2005	1/1	0.92	0.06	26,26,26,26	0
3	MG	J	2003	1/1	0.92	0.16	31,31,31,31	0
4	NA	F	2004	1/1	0.92	0.15	44,44,44,44	0
3	MG	H	2002	1/1	0.93	0.15	37,37,37,37	0
2	2FG	N	2001	11/12	0.93	0.10	33,37,43,48	0
3	MG	I	2003	1/1	0.93	0.10	33,33,33,33	0
2	2FG	O	2001	11/12	0.93	0.10	34,38,44,49	0
4	NA	O	2004	1/1	0.93	0.08	53,53,53,53	0
4	NA	F	2005	1/1	0.93	0.07	28,28,28,28	0
4	NA	G	2004	1/1	0.93	0.09	48,48,48,48	0
3	MG	A	2003	1/1	0.94	0.14	24,24,24,24	0
3	MG	C	2003	1/1	0.94	0.13	21,21,21,21	0
4	NA	E	2004	1/1	0.94	0.10	58,58,58,58	0
2	2FG	K	2001	11/12	0.94	0.10	41,45,52,56	0
3	MG	E	2002	1/1	0.94	0.08	38,38,38,38	0
3	MG	N	2002	1/1	0.94	0.10	32,32,32,32	0
3	MG	G	2002	1/1	0.94	0.15	29,29,29,29	0
4	NA	H	2004	1/1	0.94	0.08	56,56,56,56	0
2	2FG	D	2001	11/12	0.94	0.10	28,32,38,43	0
2	2FG	B	2001	11/12	0.94	0.12	23,27,34,38	0
4	NA	P	2005	1/1	0.94	0.11	51,51,51,51	0
3	MG	E	2003	1/1	0.95	0.12	39,39,39,39	0
4	NA	A	2004	1/1	0.95	0.07	44,44,44,44	0
4	NA	A	2005	1/1	0.95	0.10	28,28,28,28	0
2	2FG	G	2001	11/12	0.95	0.08	29,33,40,44	0
3	MG	M	2003	1/1	0.95	0.18	43,43,43,43	0
4	NA	C	2005	1/1	0.95	0.07	24,24,24,24	0
3	MG	A	2002	1/1	0.95	0.07	24,24,24,24	0
3	MG	K	2002	1/1	0.95	0.14	41,41,41,41	0
4	NA	E	2005	1/1	0.95	0.09	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	K	2004	1/1	0.96	0.10	60,60,60,60	0
3	MG	H	2003	1/1	0.96	0.07	37,37,37,37	0
4	NA	C	2004	1/1	0.96	0.12	41,41,41,41	0
3	MG	D	2002	1/1	0.96	0.06	27,27,27,27	0
4	NA	D	2004	1/1	0.96	0.08	47,47,47,47	0
4	NA	N	2004	1/1	0.96	0.09	52,52,52,52	0
4	NA	H	2005	1/1	0.96	0.12	40,40,40,40	0
3	MG	P	2003	1/1	0.96	0.08	48,48,48,48	0
3	MG	B	2003	1/1	0.96	0.11	23,23,23,23	0
3	MG	J	2002	1/1	0.96	0.06	30,30,30,30	0
2	2FG	C	2001	11/12	0.96	0.08	22,26,32,37	0
3	MG	B	2002	1/1	0.97	0.20	23,23,23,23	0
3	MG	N	2003	1/1	0.97	0.09	32,32,32,32	0
3	MG	O	2002	1/1	0.97	0.17	33,33,33,33	0
3	MG	L	2003	1/1	0.97	0.06	40,40,40,40	0
3	MG	G	2003	1/1	0.97	0.11	29,29,29,29	0
4	NA	L	2005	1/1	0.97	0.09	44,44,44,44	0
3	MG	F	2003	1/1	0.97	0.13	25,25,25,25	0
3	MG	C	2002	1/1	0.98	0.11	21,21,21,21	0
3	MG	F	2002	1/1	0.98	0.09	25,25,25,25	0
3	MG	K	2003	1/1	0.98	0.07	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.