



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:23 PM GMT

PDB ID : 4V40
Title : BETA-GALACTOSIDASE
Authors : Jacobson, R.H.; Zhang, X.; Dubose, R.F.; Matthews, B.W.
Deposited on : 1994-07-18
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

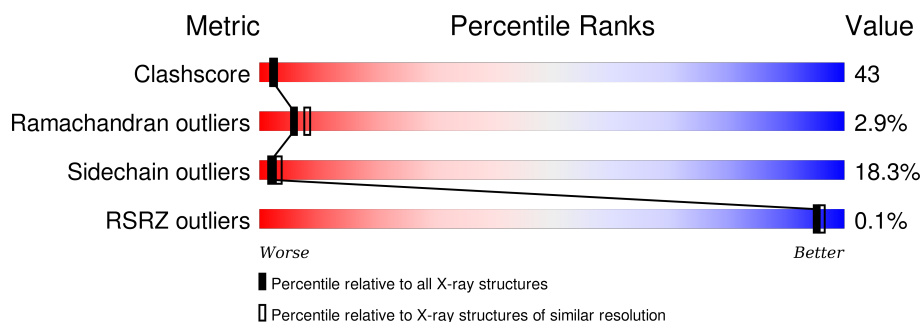
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



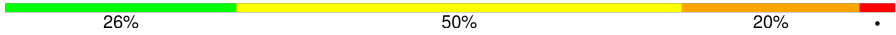
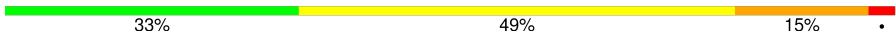



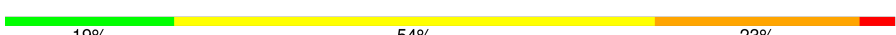
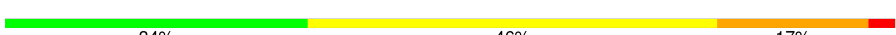
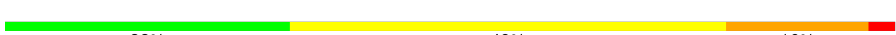

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	
1	B	1023	
1	C	1023	
1	D	1023	
1	E	1023	
1	F	1023	
1	G	1023	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
2	MG	A	1101	-	-	-	X
2	MG	B	1101	-	-	-	X
2	MG	C	1101	-	-	-	X
2	MG	D	1101	-	-	-	X
2	MG	D	1102	-	-	-	X
2	MG	E	1101	-	-	-	X
2	MG	F	1101	-	-	-	X
2	MG	G	1101	-	-	-	X
2	MG	H	1101	-	-	-	X
2	MG	I	1101	-	-	-	X
2	MG	J	1101	-	-	-	X
2	MG	L	1101	-	-	-	X
2	MG	N	1101	-	-	-	X
2	MG	O	1101	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 132654 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	0	0
			8198	5185	1451	1524	38			
1	B	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	C	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	D	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	E	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	F	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	G	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	H	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	I	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	J	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	K	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	L	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	M	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	N	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	O	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	P	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Mg 2	0	0
2	G	2	Total 2	Mg 2	0	0
2	J	2	Total 2	Mg 2	0	0
2	D	2	Total 2	Mg 2	0	0
2	K	2	Total 2	Mg 2	0	0
2	E	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	I	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	O	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	96	Total 96	O 96	0	0
3	C	91	Total 91	O 91	0	0

Continued on next page...

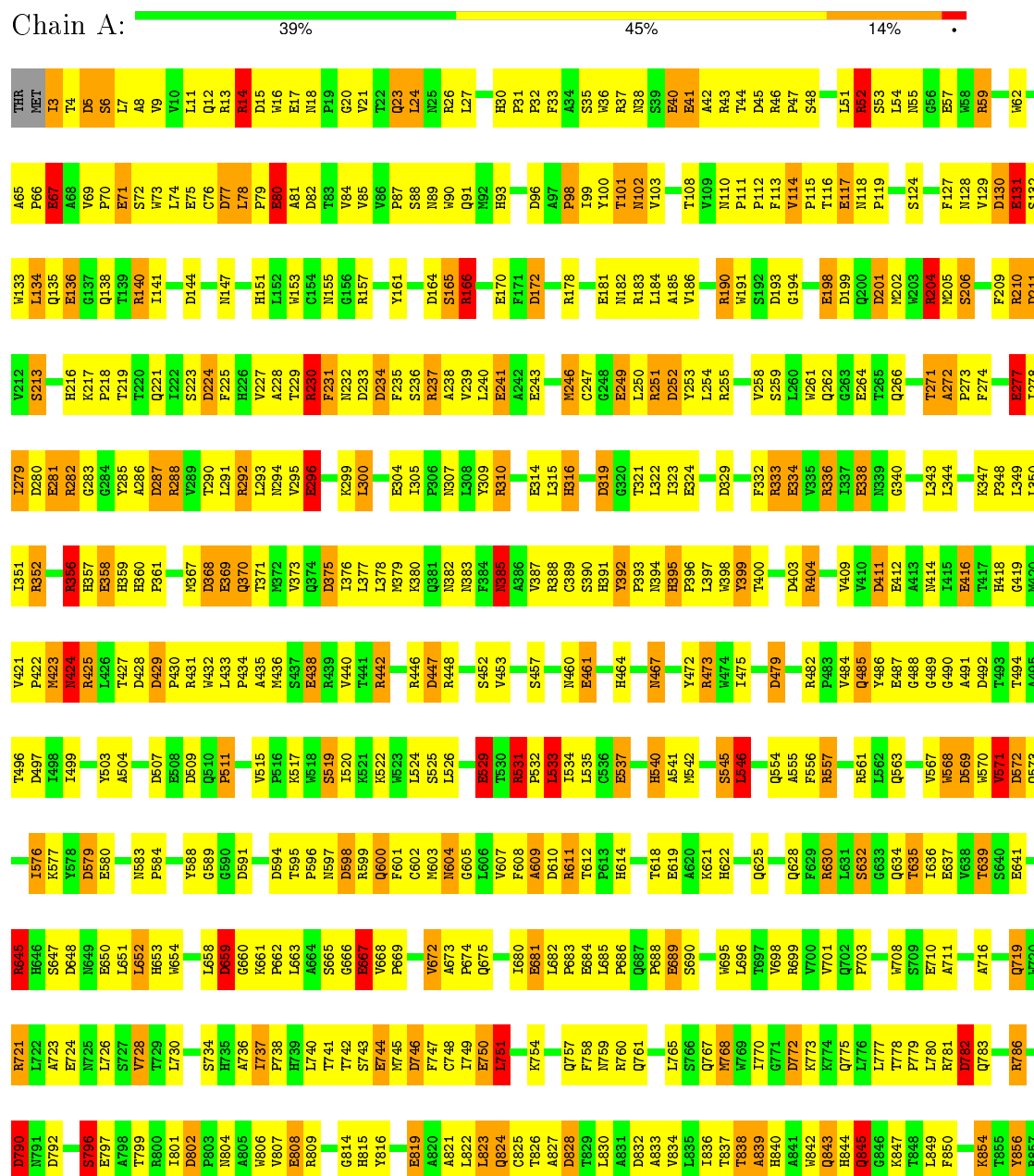
Continued from previous page...

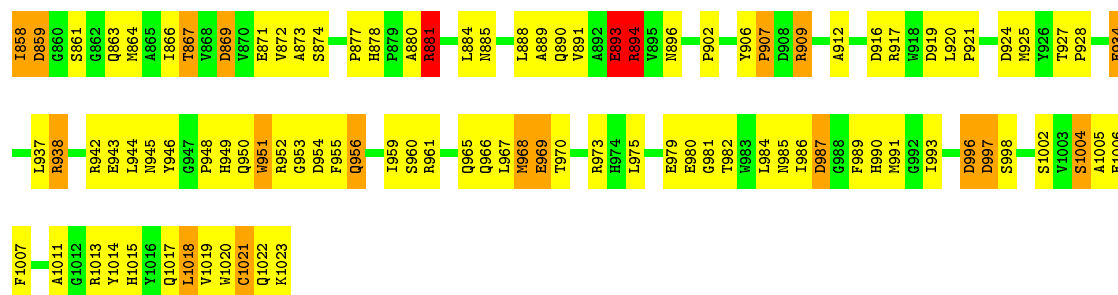
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total 97	O 97	0	0
3	E	94	Total 94	O 94	0	0
3	F	91	Total 91	O 91	0	0
3	G	95	Total 95	O 95	0	0
3	H	92	Total 92	O 92	0	0
3	I	90	Total 90	O 90	0	0
3	J	97	Total 97	O 97	0	0
3	K	87	Total 87	O 87	0	0
3	L	84	Total 84	O 84	0	0
3	M	79	Total 79	O 79	0	0
3	N	94	Total 94	O 94	0	0
3	O	95	Total 95	O 95	0	0
3	P	85	Total 85	O 85	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

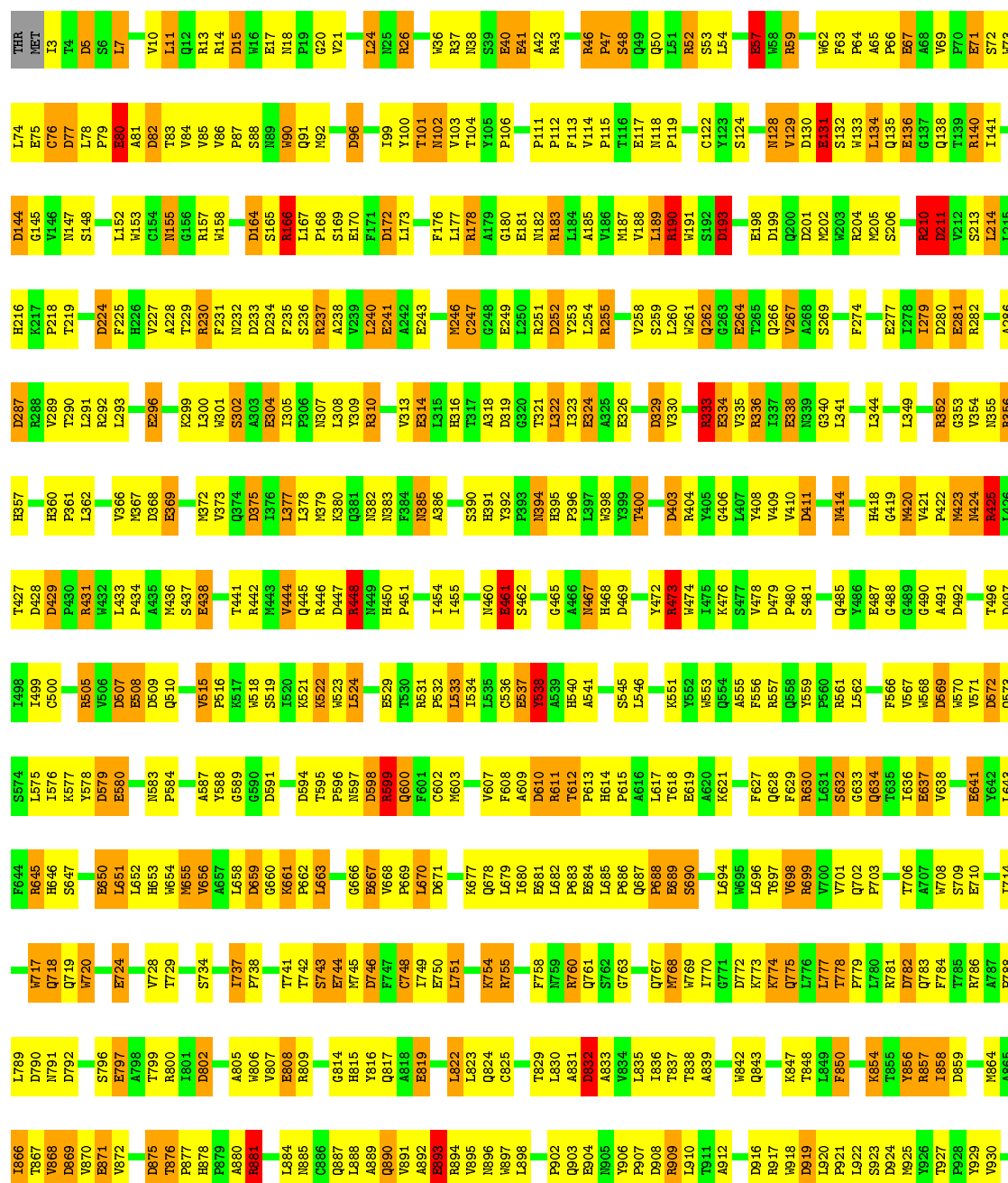
• Molecule 1: BETA-GALACTOSIDASE

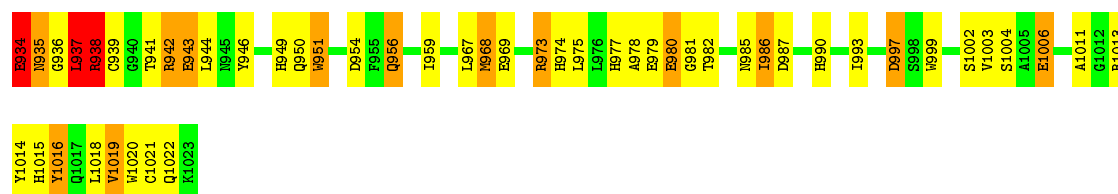




• Molecule 1: BETA-GALACTOSIDASE

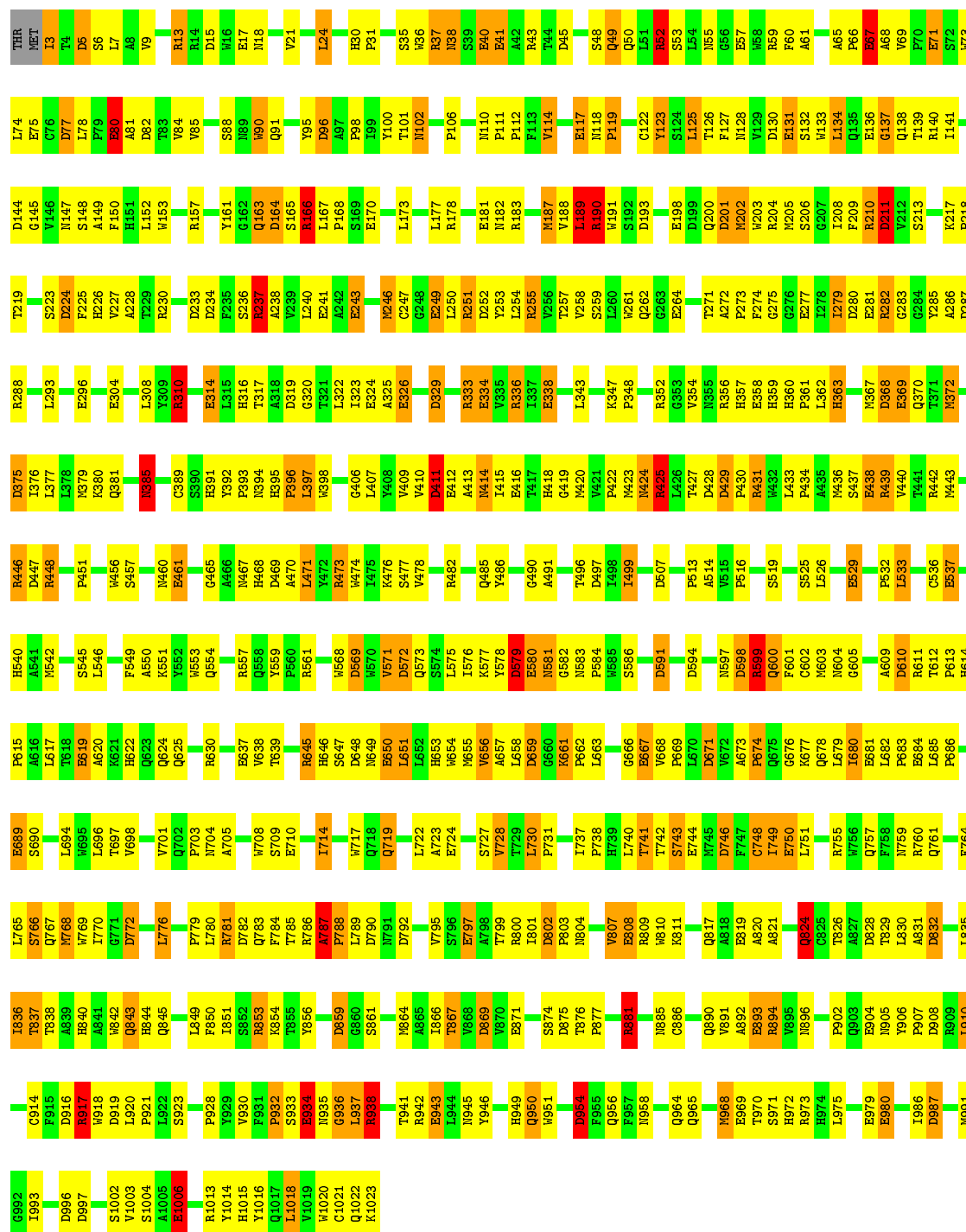
Chain B: 38% 43% 16%



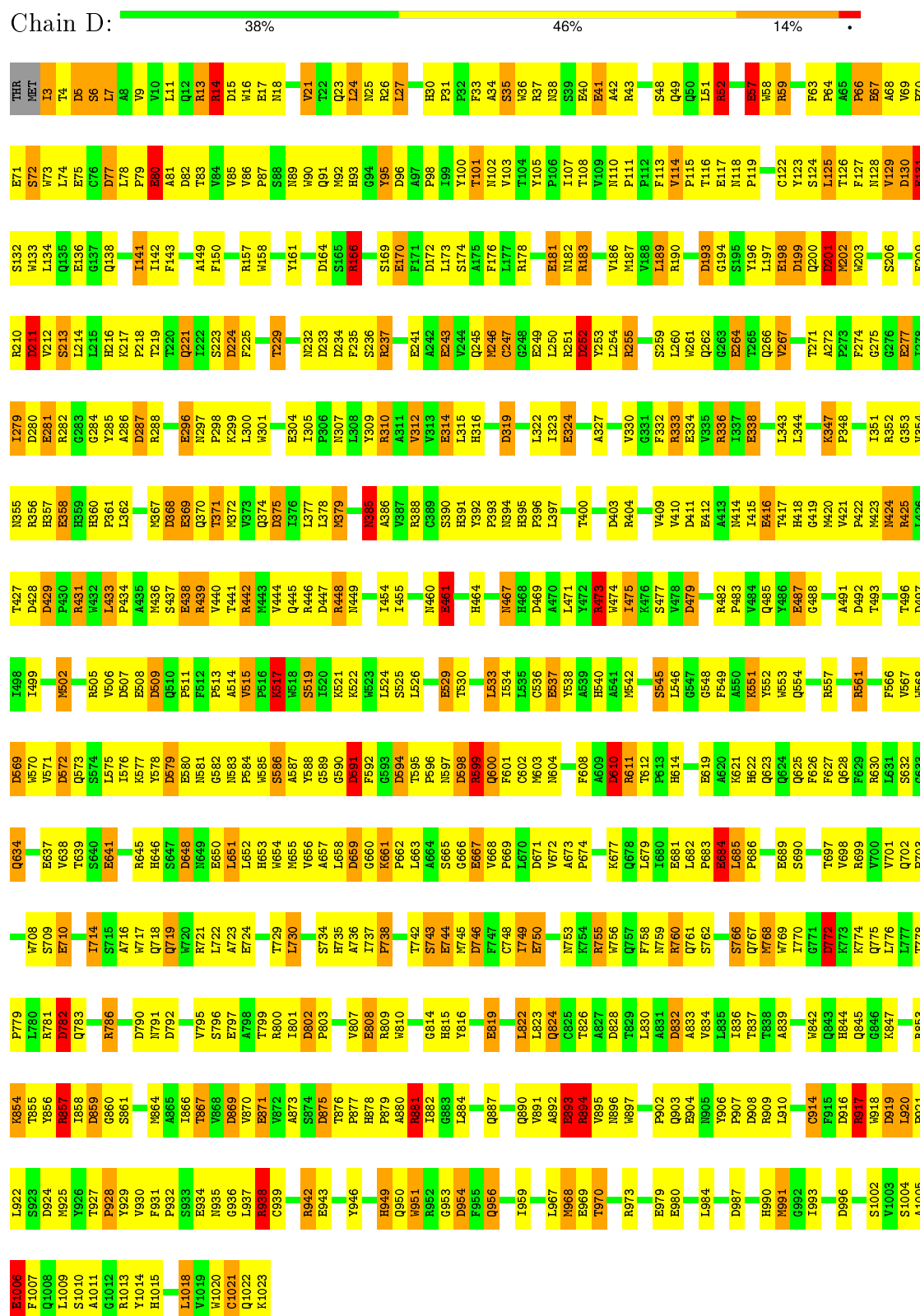


• Molecule 1: BETA-GALACTOSIDASE

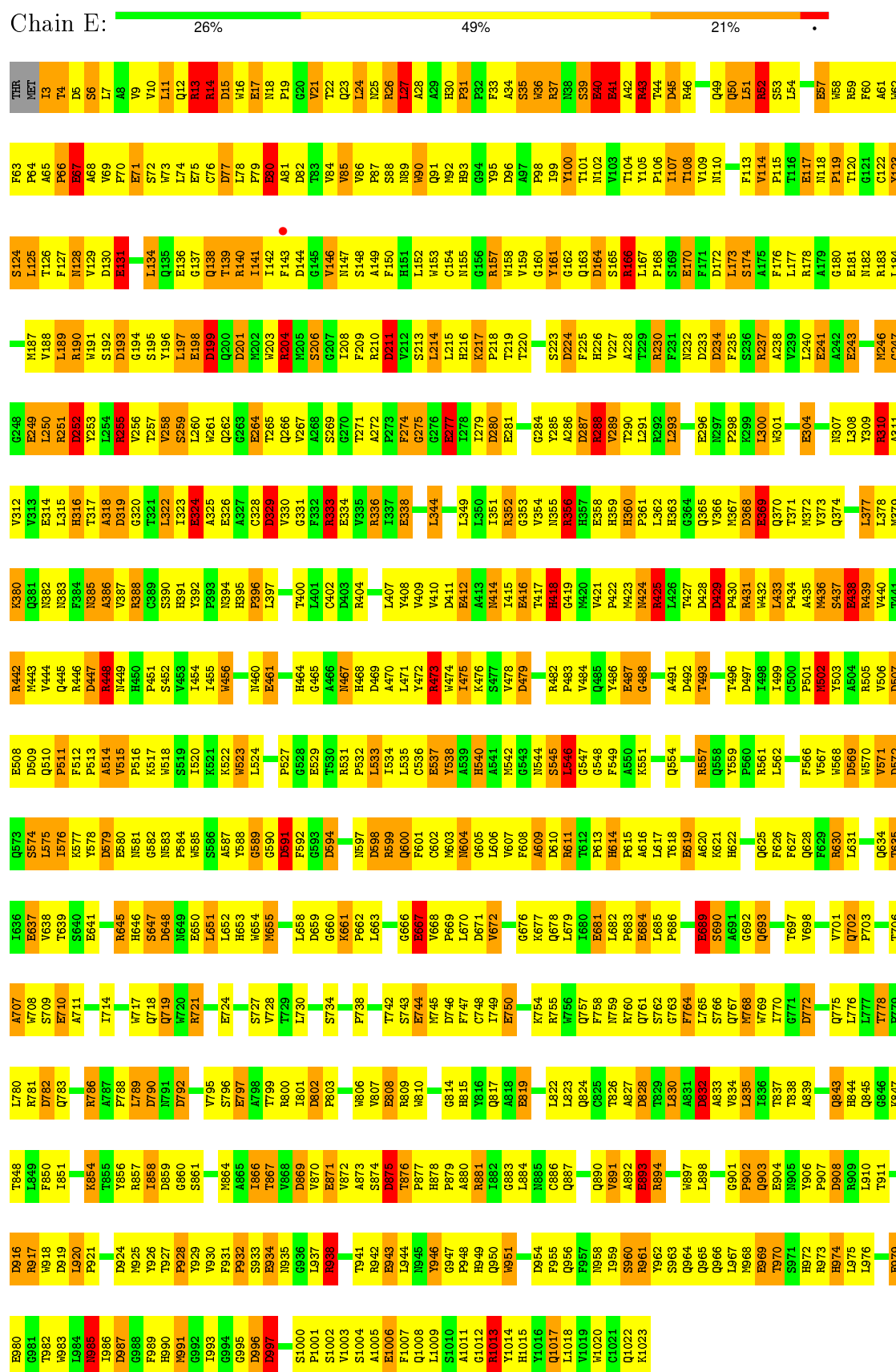
Chain C: 44% 41% 12%



• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE

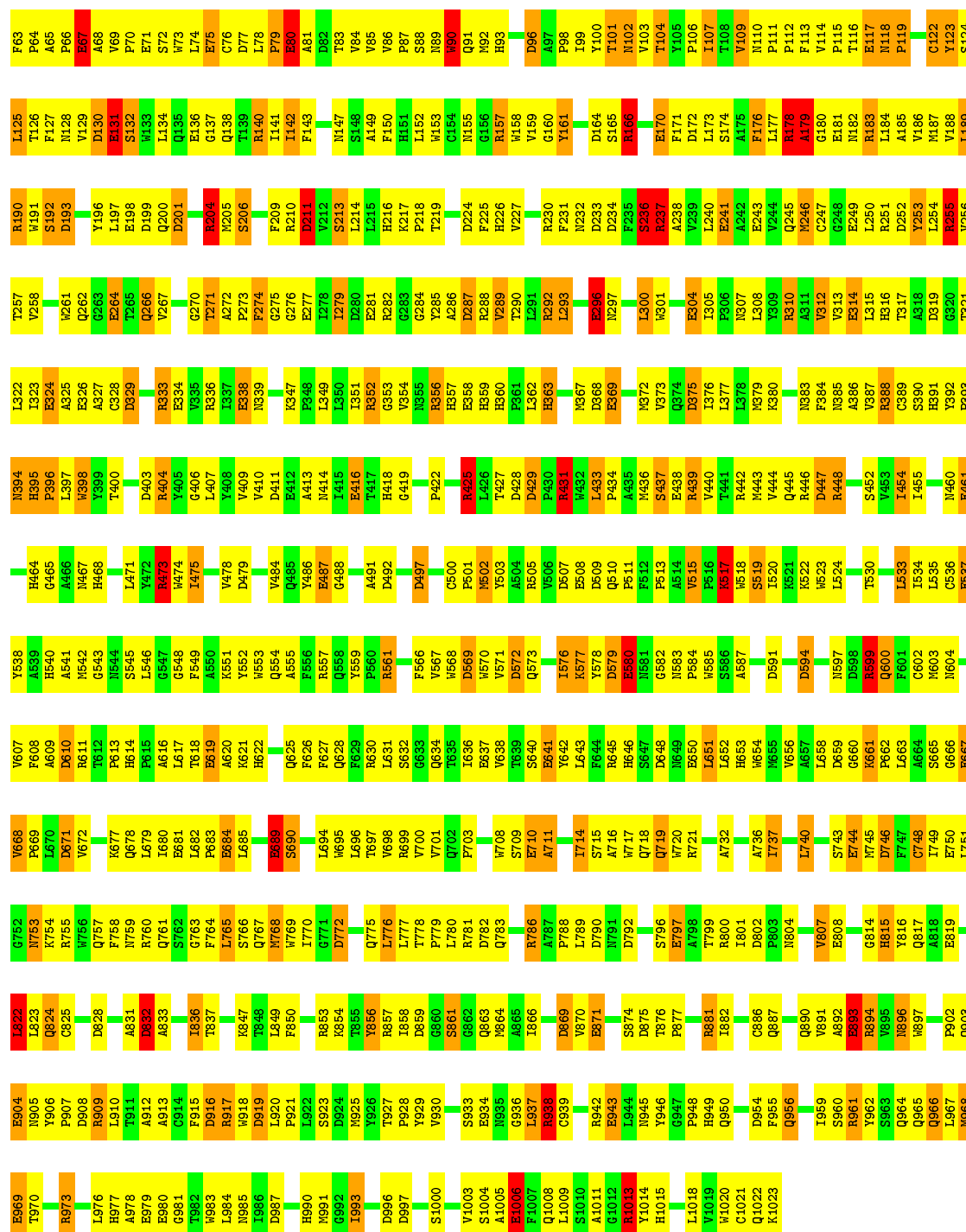


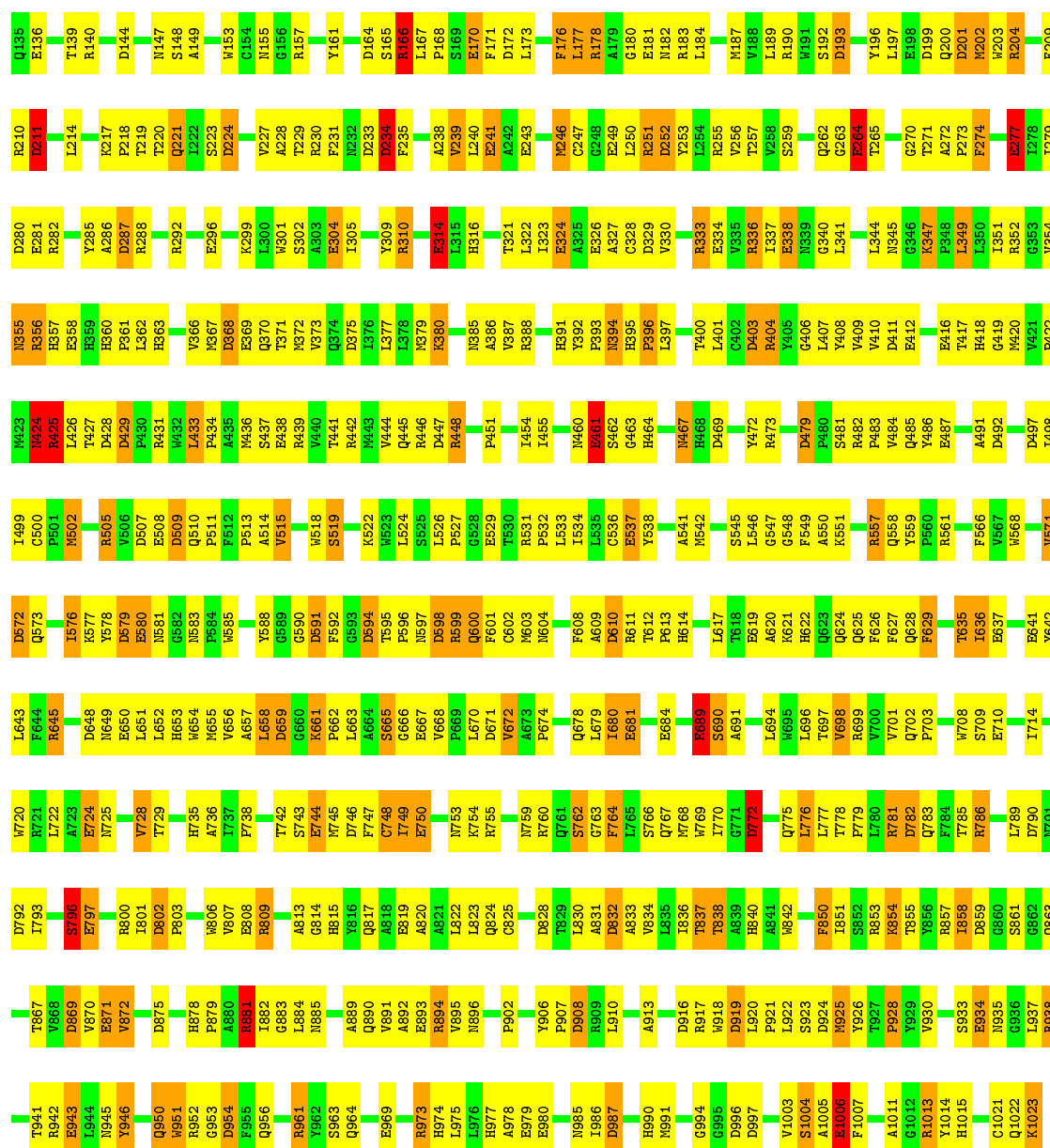




Response	Percentage
Yes	33%
No	49%
Don't know	15%

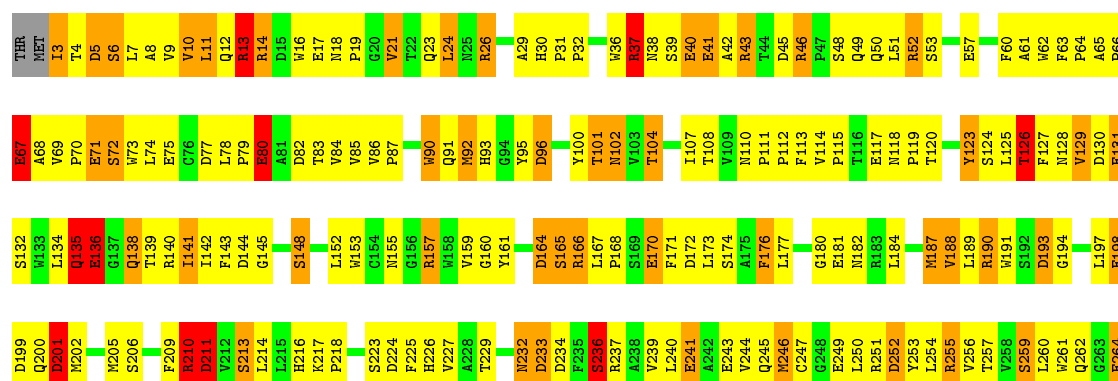


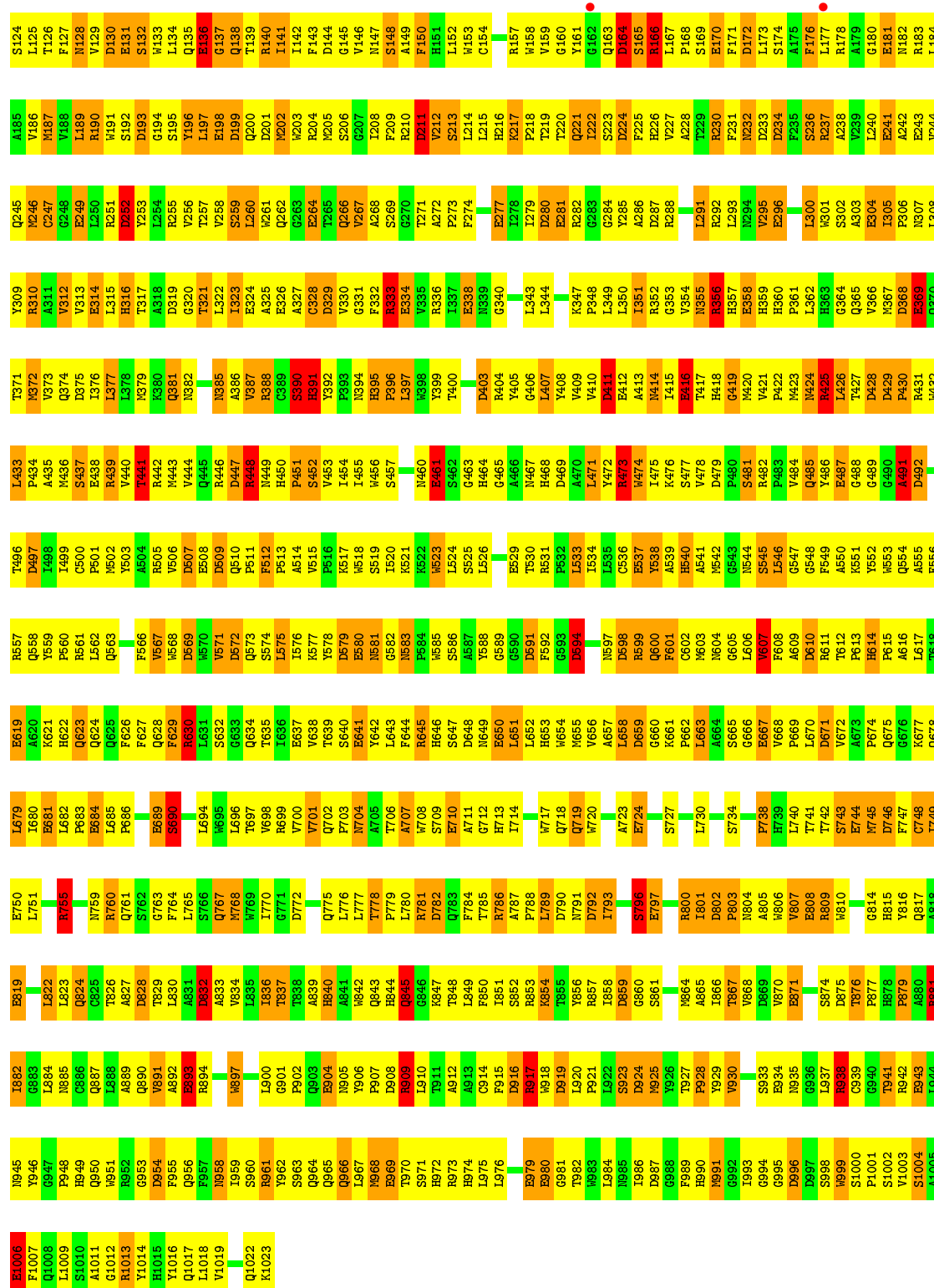




• Molecule 1: BETA-GALACTOSIDASE

Chain K: 30% 50% 16%

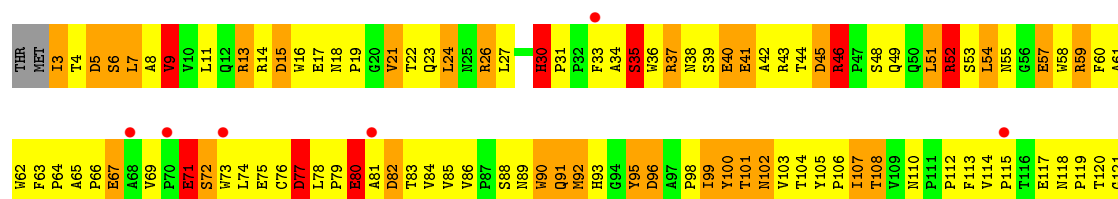




Molecule 1: BETA-GALACTOSIDASE

Chain N:





F1007	R942	B881	H815	N753	L685	Q623	Y559	G490	P430	D368	N307	Q245	A185	G122
Q1008	E943	L284	Y816	K754	P666	Q624	P660	A491	R631	E369	L308	P246	Y186	Y123
L1009	I944	B885	Q817	R755	Q887	R625	R561	D492	W432	Q370	Y309	C247	M187	
S1010	N945	A818	A818		P688	F626	L562	T493	L433		R310	G248	T126	T126
	Y946	Q866	E819	N758	S890	F629	Q563	T494	P434	Q373	A311	E249	F127	
R1013	G947	Q867	L822	T759	E899	R630	F566	A495	A435	Q374	N312	R351	L189	N128
Y1014	Y1014	L883	L823	R760	L694	L631	F567	T496	N436	D375	V313	E251	R190	N129
H1015	L823	Q824	W895		W895	S632	W568	D497	S437	L376	E314	D282	W191	D130
Y1016	D828			F764	L696	G633	W568	T498	A438	L377	L315	Y253	D193	E131
Q1017	T829	W891	T829	L765	T897	G634	D669	C500	R439	M379	R316	L254	G194	S132
L1018	R329	W892	L830	S766	W698	T635	W571	M501	V440	K380	T317	R255	S195	W133
Y1019	L830	W893	L830	O767	R699	T636	D572	M502	T441	Q381	A318	T256	Y196	W134
H1020	R694	R894	R694	T767		L637	Q573	Y503	R443	N382	D319	T257	L197	Q135
Q1021	P955	W895	A831	M768	V700	E637	Q573	Y503	W443		G520	V258	E188	E136
Q1022	Q956	R896	D832	W769	V701	V638	S574	A504	V444	N383	T321	S259	D199	G137
K1023	P957	W897	A832	I770	Q702	T639	R505	Q445	Q445	F384	L322	L260	Q200	Q138
	N958	L898	W834	P703	P703	S646	W506	V506	R446	N385	I323	W261	T139	Q138
	Y959	G899	L835	W772	N704	E641	K577	D507	D447	A366	E324	Q262	N202	R140
S960	S960	L900	L836	K773	A705	W642	W578	E508	R448	W387	A325	G263	W203	I141
R961	R961	G901	T837	K774	T706	L643	D579	D509	W449	R388	E326	E264	I142	I142
Y962	Y962	P902	T838	Q775	A707	F644	E580		W450	C389	A327	T265	F143	F143
	Q965	Q903	A839	L776	W708	R645	N583	V515	P451	S390	C328	Q266	S206	G145
Q966	Q966	Q904	H840	L777	S709	H646	P584	W518	S452	H391	D329	V267	G207	G145
L967	L967	N905	A841	T778	E710	S647	H585	S519	V453	Y392	V330	A268	I208	V146
R973	R973	Y906	W842	P779	A711	D648	H585	I520	I454	P393	G331	S269	F209	N147
H974	H974	Q907	Q843	L780	G712	R649	S866	K521	W456	N394	P332	G270	R210	S143
L975	L975	D908	R844	R781	H713	E650	A887	K522	W456	H395	R333	T271	D211	A149
Y976	Y976	P915	Q845	D782	I714	L651	S457	G463	S462	P396	E334	A272	F150	F150
	E980	R916	R853	L726	W726	D659	N597	T530	G465	D403	L342	I278	R157	G156
G981	G981	Q913	T855	N791	N725	G660	D598	R531	A466	R404	L344	D280	W158	W158
T982	T982	D919	W856	D792	S727	K681	R599	P532	N467	L407	N345	E281	Q221	V159
	N985	P921	R857	I793	V728	P662	Q600	L533	H468	Y408	G346	E382	T222	G160
Y986	Y986	L922	L858	G794	T729	L663	F601	I534	D469	V409	K347	G283	S223	Y161
D987	D987	S923	D859	W795	L730	A664	C602	L535	A470	V410	P348	G284	D224	G162
		D924	G860	S796		S665	M603	C536	L471	D411	L349	Y285	F225	Q163
		Q925	S861	E797	H735	G666	N604	E537	W472	E412	L350	D287	A286	D164
		N925	Q862	A798	A736	E667	G605	Y538	R473	A413	L351	E288	V227	S165
		Y926	Q863	T799	I737	V688	L606	A539	W474	M414	R352	V289	A228	R166
		T927	M864	R800	P738	P669	W607	B540	L475	L415	G353		T229	E170
		P928	A865	L801	H739	L670	F608	A541	K476	E416	V354	L293	R230	F171
		Y929	L866	D802	L740	D671	A609	N542	S477	T417	N355	N294	N232	F172
		V930	T867	P803	T741	W672	D610	G543	V478	R418	R356	Y295	D233	L173
		P931	W668	N804	T742	A673	R611	N544	D479	G419	R357	E296	D234	S174
		P932	D869	A805	S743	P674	T612	S545	P480	M420	E358	N297	F235	A175
		S933	W870	R806	E744		P613	L546	S481	V421	R359	P298	S236	F176
		E934	E871	W807	M745	K677	P613	G547	R482	P422	R360	K299	R237	L177
		N935	S874	E308	D746	Q678	A616	G548	P483	M423	P361	L300	A238	R178
		G936	L679	R809	F747	L679	L617	F549	W484	N424	L362	N301	V239	A179
		S1000	D875	N810	C748	L680	T618	Q485	Q485	R425	R363	S302	L240	G180
		P1001	T876	R611	I749	E681	E619	K551	Y486	L426	G364	A303	E241	E181
		V1003	R877	R811	I749	L682	A620	W552	E987	T427	Q365	I305	A242	N182
		Q939	P877	A812	E750	L751	P683	W553	G488	D428	V366	E243	E243	E183
		S1004	H878	G814	G752	E684	H622		G489	D429	N367	P306	V244	L184

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 92.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 39.3 (92.62-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.174 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 89.5	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 590207 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	132654	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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, 0.375 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: MG

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	1.16	51/8440 (0.6%)	1.52	139/11516 (1.2%)
1	B	1.17	54/8440 (0.6%)	1.51	130/11516 (1.1%)
1	C	1.18	56/8440 (0.7%)	1.50	132/11516 (1.1%)
1	D	1.16	55/8440 (0.7%)	1.52	148/11516 (1.3%)
1	E	1.16	55/8440 (0.7%)	1.56	145/11516 (1.3%)
1	F	1.18	45/8440 (0.5%)	1.53	144/11516 (1.3%)
1	G	1.16	58/8440 (0.7%)	1.51	151/11516 (1.3%)
1	H	1.16	56/8440 (0.7%)	1.57	150/11516 (1.3%)
1	I	1.13	53/8440 (0.6%)	1.52	140/11516 (1.2%)
1	J	1.12	48/8440 (0.6%)	1.48	134/11516 (1.2%)
1	K	1.09	53/8440 (0.6%)	1.45	115/11516 (1.0%)
1	L	1.13	53/8440 (0.6%)	1.54	134/11516 (1.2%)
1	M	1.16	55/8440 (0.7%)	1.58	142/11516 (1.2%)
1	N	1.14	51/8440 (0.6%)	1.49	127/11516 (1.1%)
1	O	1.11	54/8440 (0.6%)	1.49	141/11516 (1.2%)
1	P	1.17	57/8440 (0.7%)	1.60	151/11516 (1.3%)
All	All	1.15	854/135040 (0.6%)	1.52	2223/184256 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	D	2	1
1	E	1	0
1	F	2	0
1	G	2	0
1	H	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	1	0
1	J	1	0
1	L	1	0
1	M	2	0
1	P	2	0
All	All	17	1

The worst 5 of 854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	358	GLU	CD-OE2	11.52	1.38	1.25
1	F	75	GLU	CD-OE1	10.30	1.36	1.25
1	K	358	GLU	CD-OE2	9.34	1.35	1.25
1	B	650	GLU	CD-OE1	9.31	1.35	1.25
1	F	326	GLU	CD-OE2	9.01	1.35	1.25

The worst 5 of 2223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	B	166	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	N	561	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	L	425	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	L	997	ASP	CB-CG-OD2	-13.64	106.02	118.30

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	TRP	CA
1	B	718	GLN	CA
1	D	95	TYR	CA
1	D	914	CYS	CA
1	E	118	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	ARG	Sidechain

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	8198	0	7796	540	0
1	B	8198	0	7796	546	0
1	C	8198	0	7796	446	0
1	D	8198	0	7796	551	0
1	E	8198	0	7795	892	0
1	F	8198	0	7796	579	0
1	G	8198	0	7796	641	0
1	H	8198	0	7796	882	0
1	I	8198	0	7796	618	0
1	J	8198	0	7795	507	0
1	K	8198	0	7796	781	0
1	L	8198	0	7796	792	0
1	M	8198	0	7796	1078	0
1	N	8198	0	7795	630	0
1	O	8198	0	7796	659	0
1	P	8198	0	7796	1151	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	88	0	0	7	0
3	B	96	0	0	14	0
3	C	91	0	0	9	0
3	D	97	0	0	13	0
3	E	94	0	0	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	91	0	0	9	0
3	G	95	0	0	13	0
3	H	92	0	0	18	0
3	I	90	0	0	15	0
3	J	97	0	0	9	0
3	K	87	0	0	9	0
3	L	84	0	0	12	0
3	M	79	0	0	17	0
3	N	94	0	0	19	0
3	O	95	0	0	12	0
3	P	85	0	0	21	0
All	All	132654	0	124733	11096	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 11096 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LEU:HD13	1:E:74:LEU:HD11	1.23	1.17
1:D:572:ASP:HB3	1:D:603:MET:HG2	1.25	1.16
1:C:427:THR:HA	1:C:436:MET:HE1	1.21	1.16
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.18	1.15
1:I:316:HIS:HA	1:I:323:ILE:HD13	1.24	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1019/1023 (100%)	909 (89%)	92 (9%)	18 (2%)	11 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1019/1023 (100%)	914 (90%)	85 (8%)	20 (2%)	9	15
1	C	1019/1023 (100%)	919 (90%)	81 (8%)	19 (2%)	10	16
1	D	1019/1023 (100%)	910 (89%)	98 (10%)	11 (1%)	17	31
1	E	1019/1023 (100%)	842 (83%)	135 (13%)	42 (4%)	3	4
1	F	1019/1023 (100%)	892 (88%)	101 (10%)	26 (3%)	7	10
1	G	1019/1023 (100%)	893 (88%)	101 (10%)	25 (2%)	7	10
1	H	1019/1023 (100%)	845 (83%)	140 (14%)	34 (3%)	5	6
1	I	1019/1023 (100%)	884 (87%)	111 (11%)	24 (2%)	7	11
1	J	1019/1023 (100%)	887 (87%)	118 (12%)	14 (1%)	14	24
1	K	1019/1023 (100%)	855 (84%)	131 (13%)	33 (3%)	5	6
1	L	1019/1023 (100%)	838 (82%)	146 (14%)	35 (3%)	5	6
1	M	1019/1023 (100%)	836 (82%)	127 (12%)	56 (6%)	2	2
1	N	1019/1023 (100%)	875 (86%)	117 (12%)	27 (3%)	7	10
1	O	1019/1023 (100%)	889 (87%)	102 (10%)	28 (3%)	6	9
1	P	1019/1023 (100%)	797 (78%)	164 (16%)	58 (6%)	2	2
All	All	16304/16368 (100%)	13985 (86%)	1849 (11%)	470 (3%)	6	8

5 of 470 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	277	GLU
1	A	389	CYS
1	A	541	ALA
1	A	659	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	873/875 (100%)	723 (83%)	150 (17%)	2 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	873/875 (100%)	709 (81%)	164 (19%)	2	3
1	C	873/875 (100%)	754 (86%)	119 (14%)	5	8
1	D	873/875 (100%)	729 (84%)	144 (16%)	3	5
1	E	873/875 (100%)	686 (79%)	187 (21%)	1	2
1	F	873/875 (100%)	735 (84%)	138 (16%)	3	5
1	G	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	H	873/875 (100%)	693 (79%)	180 (21%)	1	2
1	I	873/875 (100%)	716 (82%)	157 (18%)	2	3
1	J	873/875 (100%)	755 (86%)	118 (14%)	5	9
1	K	873/875 (100%)	722 (83%)	151 (17%)	2	4
1	L	873/875 (100%)	704 (81%)	169 (19%)	2	3
1	M	873/875 (100%)	677 (78%)	196 (22%)	1	1
1	N	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	O	873/875 (100%)	715 (82%)	158 (18%)	2	3
1	P	873/875 (100%)	665 (76%)	208 (24%)	1	1
All	All	13968/14000 (100%)	11417 (82%)	2551 (18%)	2	3

5 of 2551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	523	TRP
1	J	277	GLU
1	P	71	GLU
1	H	724	GLU
1	I	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	262	GLN
1	I	950	GLN
1	O	1008	GLN
1	H	460	ASN
1	I	38	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1021/1023 (99%)	-1.05	0 100 100	2, 24, 54, 79	0
1	B	1021/1023 (99%)	-1.08	0 100 100	2, 23, 54, 81	0
1	C	1021/1023 (99%)	-1.04	0 100 100	4, 21, 52, 80	0
1	D	1021/1023 (99%)	-1.08	0 100 100	4, 25, 56, 81	0
1	E	1021/1023 (99%)	-0.92	1 (0%) 95 96	8, 34, 61, 86	0
1	F	1021/1023 (99%)	-1.01	0 100 100	2, 23, 55, 78	0
1	G	1021/1023 (99%)	-1.05	0 100 100	3, 27, 58, 82	0
1	H	1021/1023 (99%)	-0.90	1 (0%) 95 96	6, 33, 61, 89	0
1	I	1021/1023 (99%)	-1.00	0 100 100	4, 30, 59, 80	0
1	J	1021/1023 (99%)	-1.00	0 100 100	8, 28, 56, 85	0
1	K	1021/1023 (99%)	-0.86	1 (0%) 95 96	10, 35, 64, 92	0
1	L	1021/1023 (99%)	-0.83	1 (0%) 95 96	6, 35, 63, 84	0
1	M	1021/1023 (99%)	-0.77	3 (0%) 94 95	12, 39, 65, 80	0
1	N	1021/1023 (99%)	-0.94	0 100 100	9, 30, 59, 89	0
1	O	1021/1023 (99%)	-0.98	0 100 100	11, 31, 60, 81	0
1	P	1021/1023 (99%)	-0.42	17 (1%) 73 76	14, 43, 69, 89	0
All	All	16336/16368 (99%)	-0.93	24 (0%) 95 96	2, 30, 60, 92	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	81	ALA	4.3
1	P	313	VAL	3.6
1	P	143	PHE	3.4
1	P	70	PRO	3.3
1	P	141	ILE	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	1101	1/1	0.98	0.15	13.18	37,37,37,37	0
2	MG	F	1101	1/1	0.78	0.19	12.48	35,35,35,35	0
2	MG	C	1101	1/1	0.97	0.18	11.03	23,23,23,23	0
2	MG	G	1101	1/1	0.91	0.17	9.44	32,32,32,32	0
2	MG	B	1101	1/1	0.96	0.15	6.04	25,25,25,25	0
2	MG	I	1101	1/1	0.99	0.13	5.76	33,33,33,33	0
2	MG	N	1101	1/1	0.97	0.14	4.50	32,32,32,32	0
2	MG	H	1101	1/1	0.96	0.15	3.80	27,27,27,27	0
2	MG	J	1101	1/1	0.94	0.14	3.71	34,34,34,34	0
2	MG	D	1102	1/1	0.95	0.13	3.38	42,42,42,42	0
2	MG	E	1101	1/1	0.96	0.15	3.33	39,39,39,39	0
2	MG	O	1101	1/1	0.92	0.12	2.59	40,40,40,40	0
2	MG	D	1101	1/1	0.97	0.12	2.34	28,28,28,28	0
2	MG	L	1101	1/1	0.98	0.14	2.33	31,31,31,31	0
2	MG	M	1101	1/1	0.94	0.14	1.54	56,56,56,56	0
2	MG	N	1102	1/1	0.98	0.11	0.18	26,26,26,26	0
2	MG	C	1102	1/1	0.93	0.08	-0.01	28,28,28,28	0
2	MG	P	1101	1/1	0.93	0.12	-0.29	49,49,49,49	0
2	MG	I	1102	1/1	0.98	0.08	-0.45	33,33,33,33	0
2	MG	E	1102	1/1	0.95	0.08	-0.52	32,32,32,32	0
2	MG	A	1102	1/1	0.95	0.08	-0.56	37,37,37,37	0
2	MG	K	1101	1/1	0.89	0.08	-0.70	34,34,34,34	0
2	MG	O	1102	1/1	0.99	0.09	-0.82	15,15,15,15	0
2	MG	H	1102	1/1	0.99	0.06	-1.23	22,22,22,22	0
2	MG	L	1102	1/1	0.95	0.04	-1.70	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	K	1102	1/1	0.98	0.05	-1.78	25,25,25,25	0
2	MG	F	1102	1/1	0.99	0.07	-1.93	26,26,26,26	0
2	MG	J	1102	1/1	0.96	0.05	-2.47	29,29,29,29	0
2	MG	B	1102	1/1	0.99	0.05	-2.56	23,23,23,23	0
2	MG	P	1102	1/1	0.99	0.05	-2.62	26,26,26,26	0
2	MG	G	1102	1/1	0.99	0.03	-5.22	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.