



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 05:26 PM EST

PDB ID : 4V41  
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-MONOCLINIC)  
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.  
Deposited on : 2000-06-07  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

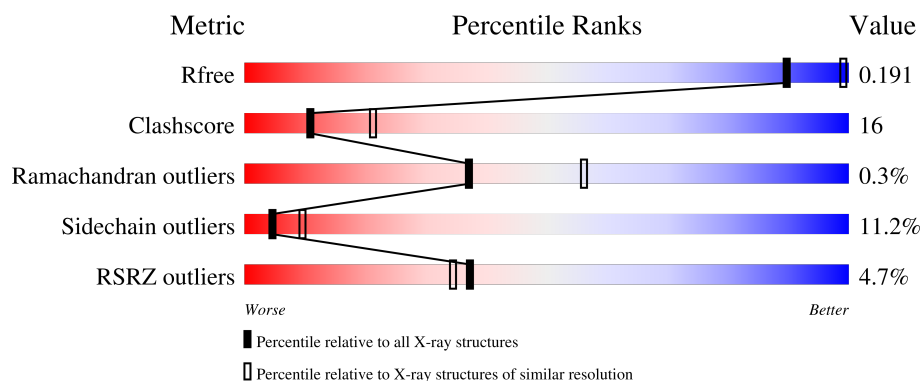
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div>59%</div> <div>30%</div> <div>9%</div> <div>.</div> </div>
1	B	1023	<div> <div>4%</div> <div>58%</div> <div>31%</div> <div>9%</div> <div>.</div> </div>
1	C	1023	<div> <div>3%</div> <div>57%</div> <div>31%</div> <div>9%</div> <div>.</div> </div>
1	D	1023	<div> <div>4%</div> <div>58%</div> <div>30%</div> <div>9%</div> <div>.</div> </div>
1	E	1023	<div> <div>4%</div> <div>58%</div> <div>30%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1023	<div><div></div><div>3%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	G	1023	<div><div></div><div>2%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	H	1023	<div><div></div><div>3%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	I	1023	<div><div></div><div>2%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	J	1023	<div><div></div><div>3%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	K	1023	<div><div></div><div>%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	L	1023	<div><div></div><div>2%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	M	1023	<div><div></div><div>14%</div><div>59%</div><div>30%</div><div>9%</div><div></div></div>
1	N	1023	<div><div></div><div>2%</div><div>58%</div><div>30%</div><div>9%</div><div></div></div>
1	O	1023	<div><div></div><div>2%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>
1	P	1023	<div><div></div><div>23%</div><div>58%</div><div>31%</div><div>9%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 138704 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	5	0
			8232	5201	1462	1528	41			
1	B	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	C	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	D	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	E	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	F	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	G	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	H	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	I	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	J	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	K	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	L	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	M	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	N	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	O	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	P	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	434	Total O 434 434	0	0
3	B	436	Total O 436 436	0	0
3	C	433	Total O 433 433	0	0
3	D	437	Total O 437 437	0	0
3	E	435	Total O 435 435	0	0
3	F	436	Total O 436 436	0	0
3	G	434	Total O 434 434	0	0
3	H	435	Total O 435 435	0	0
3	I	434	Total O 434 434	0	0
3	J	436	Total O 436 436	0	0
3	K	435	Total O 435 435	0	0
3	L	435	Total O 435 435	0	0
3	M	434	Total O 434 434	0	0
3	N	436	Total O 436 436	0	0
3	O	433	Total O 433 433	0	0
3	P	437	Total O 437 437	0	0



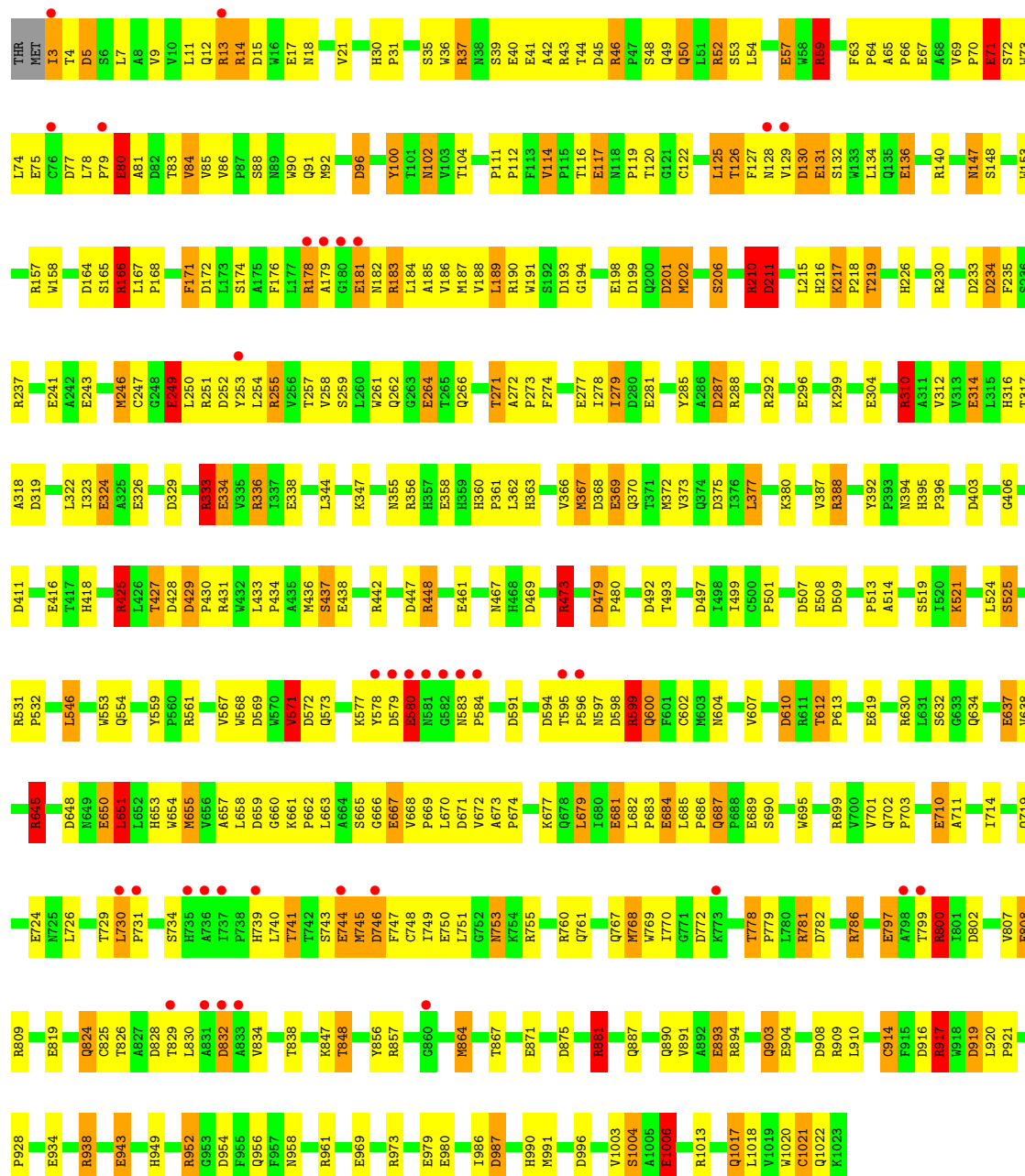
- Molecule 1: BETA-GALACTOSIDASE







• Molecule 1: BETA-GALACTOSIDASE



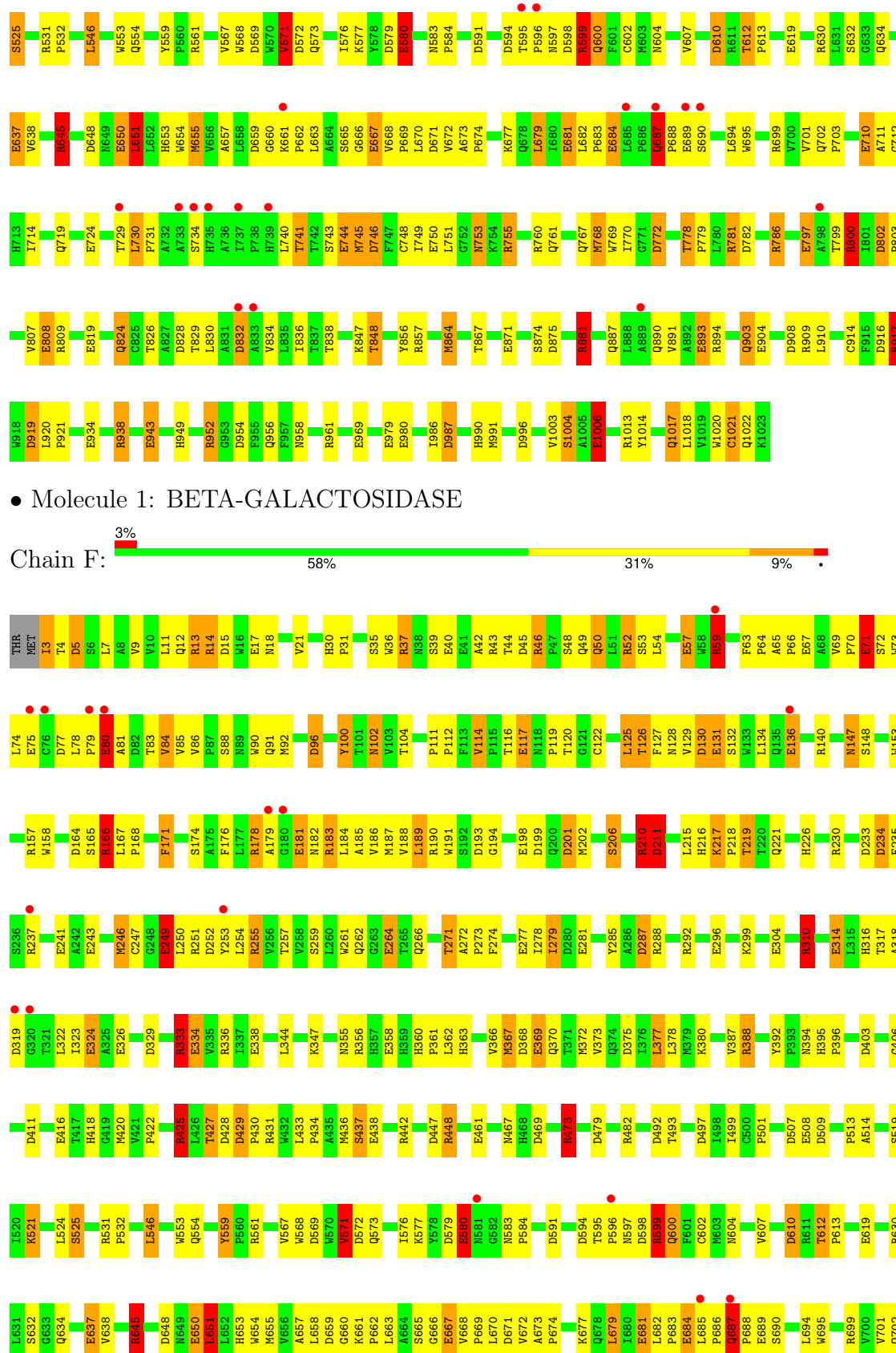
• Molecule 1: BETA-GALACTOSIDASE

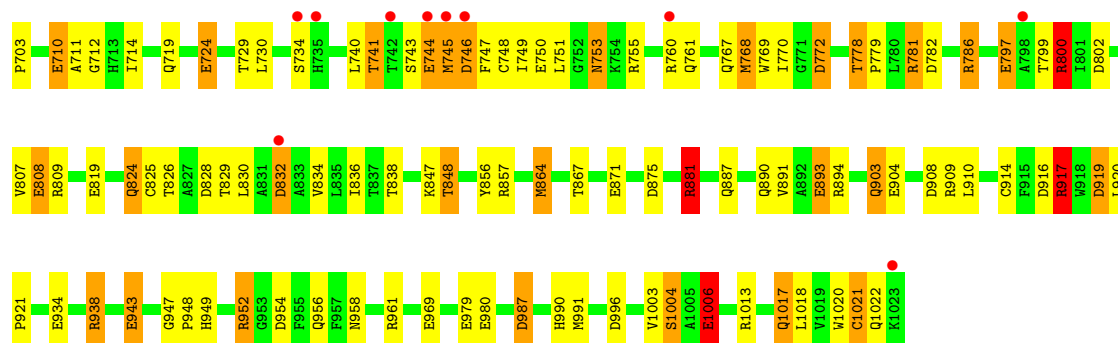




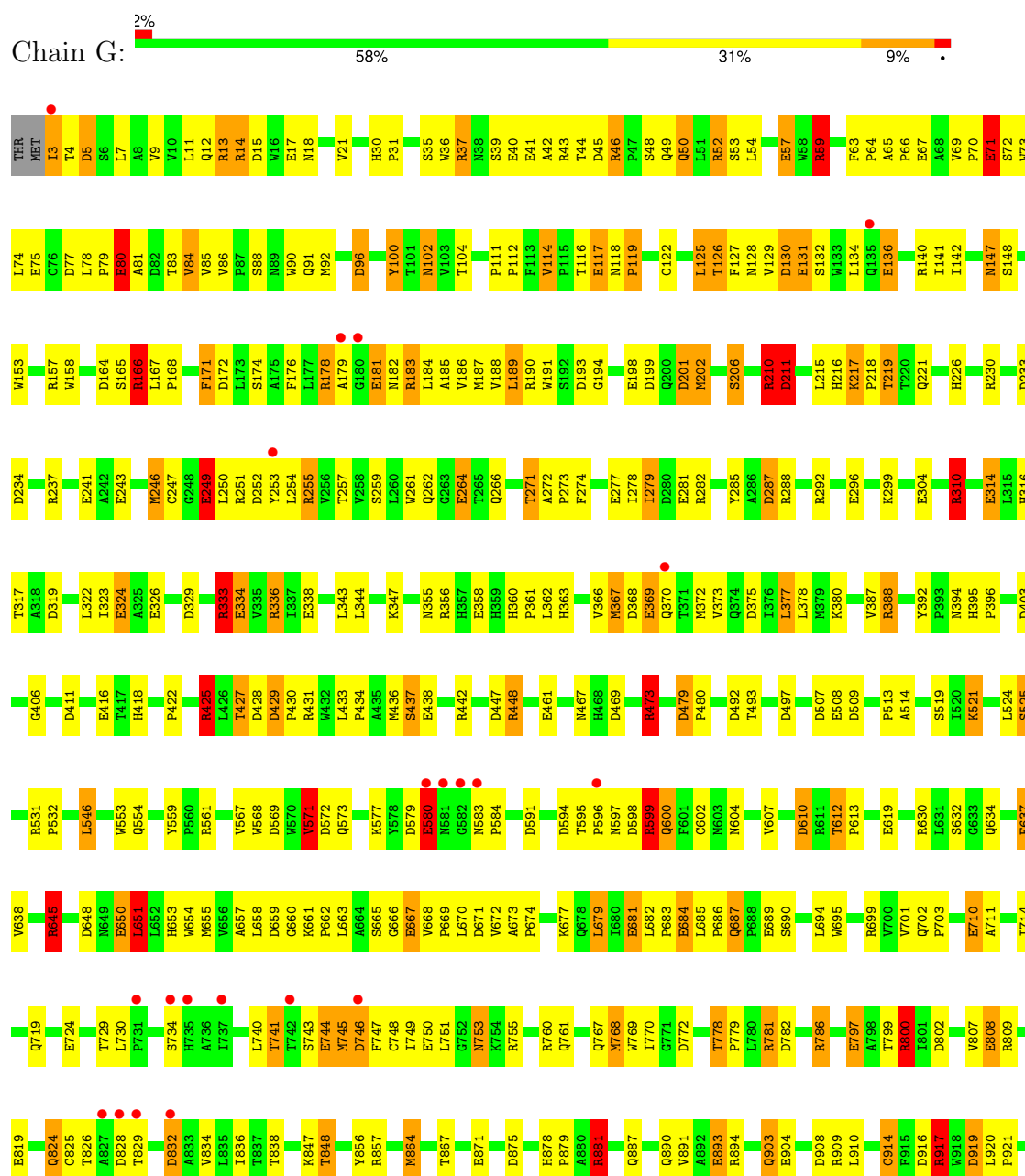
L167	L74	THR
P168	E76	MEI
S169	T75	I3
E170	T78	T4
F171	L77	D5
E172	P79	S6
L173	E80	L7
S174	A81	A8
A175	D82	V9
F176	T83	V10
L177	H84	L11
A178	H85	Q12
A179	H86	R13
G180	P87	R14
G181	S88	D15
N182	H89	A16
R183	K90	E17
L184	Q91	M18
A185	M92	
V186		V21
M187	D96	
V188		H30
L189	Y100	P31
R190	T101	
W191	M102	S35
S192	V103	V36
D193	T104	R37
G194		H38
	V114	S39
E198	P115	E40
D199	T116	E41
Q200	E117	A42
D201	M118	R43
M202	P119	T44
		D45
S206	C122	R46
		P47
R210	L125	S48
D211	T126	Q49
	F127	R50
L215	N128	L51
H216	V129	A52
K217	D130	S53
P218	E131	A54
T219	S132	L54
T220	A133	
Q221	L134	E57
	G135	A58
H226	E136	R59
R230	R140	F63
D233	M147	A65
D234	S148	P66
F235	R157	E67
S236		A68
R237		V69
		P70
E241	D164	E71
E242	S165	S72
	R168	T72





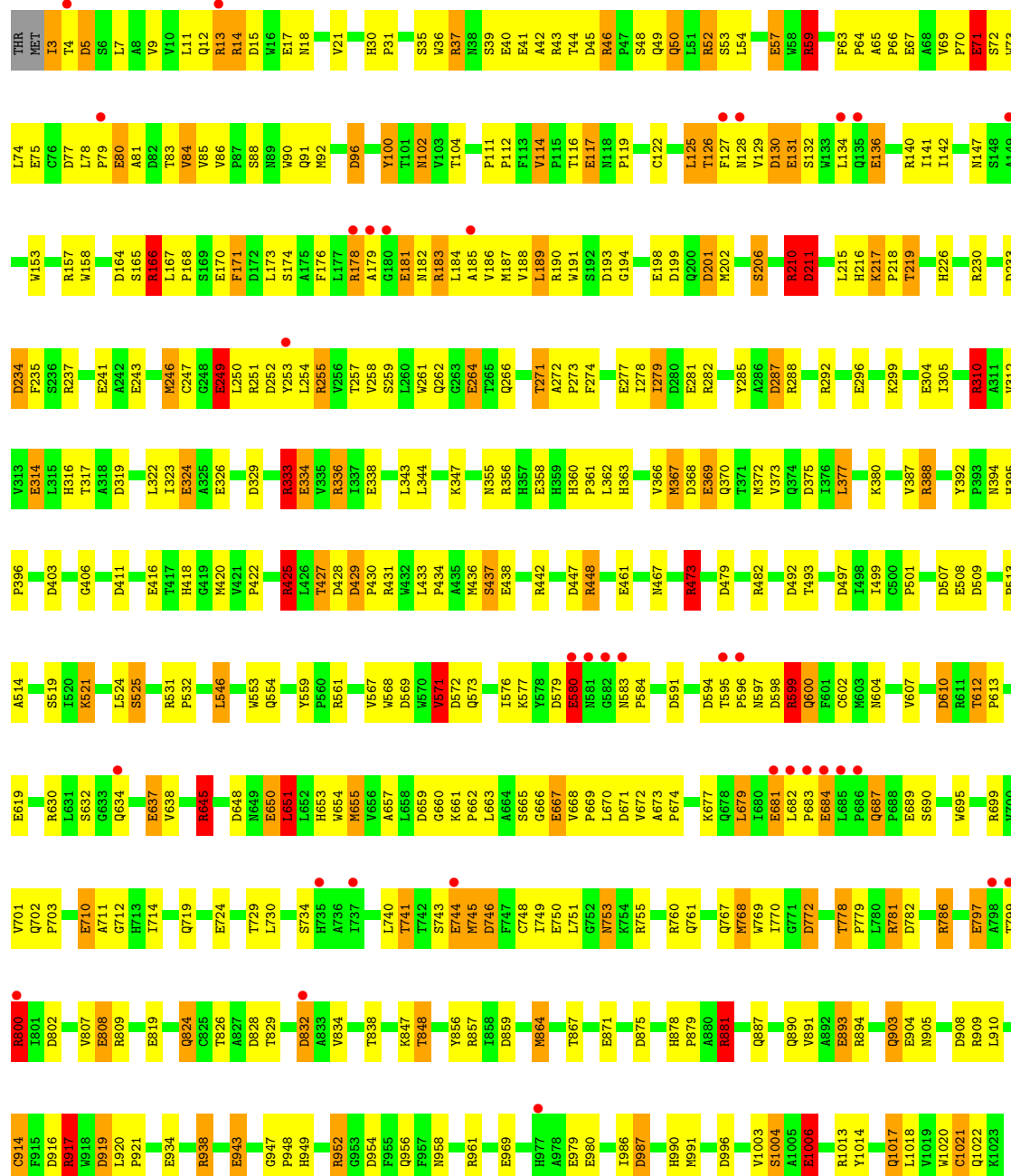


• Molecule 1: BETA-GALACTOSIDASE



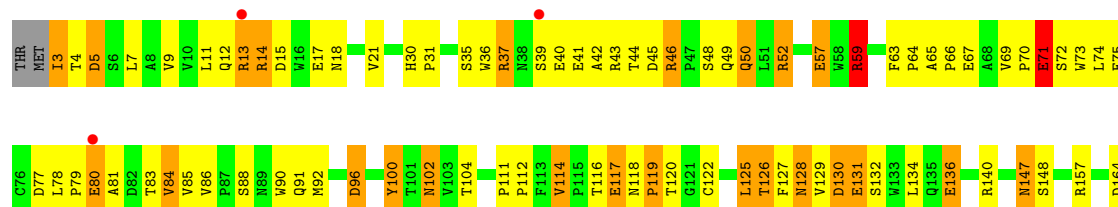


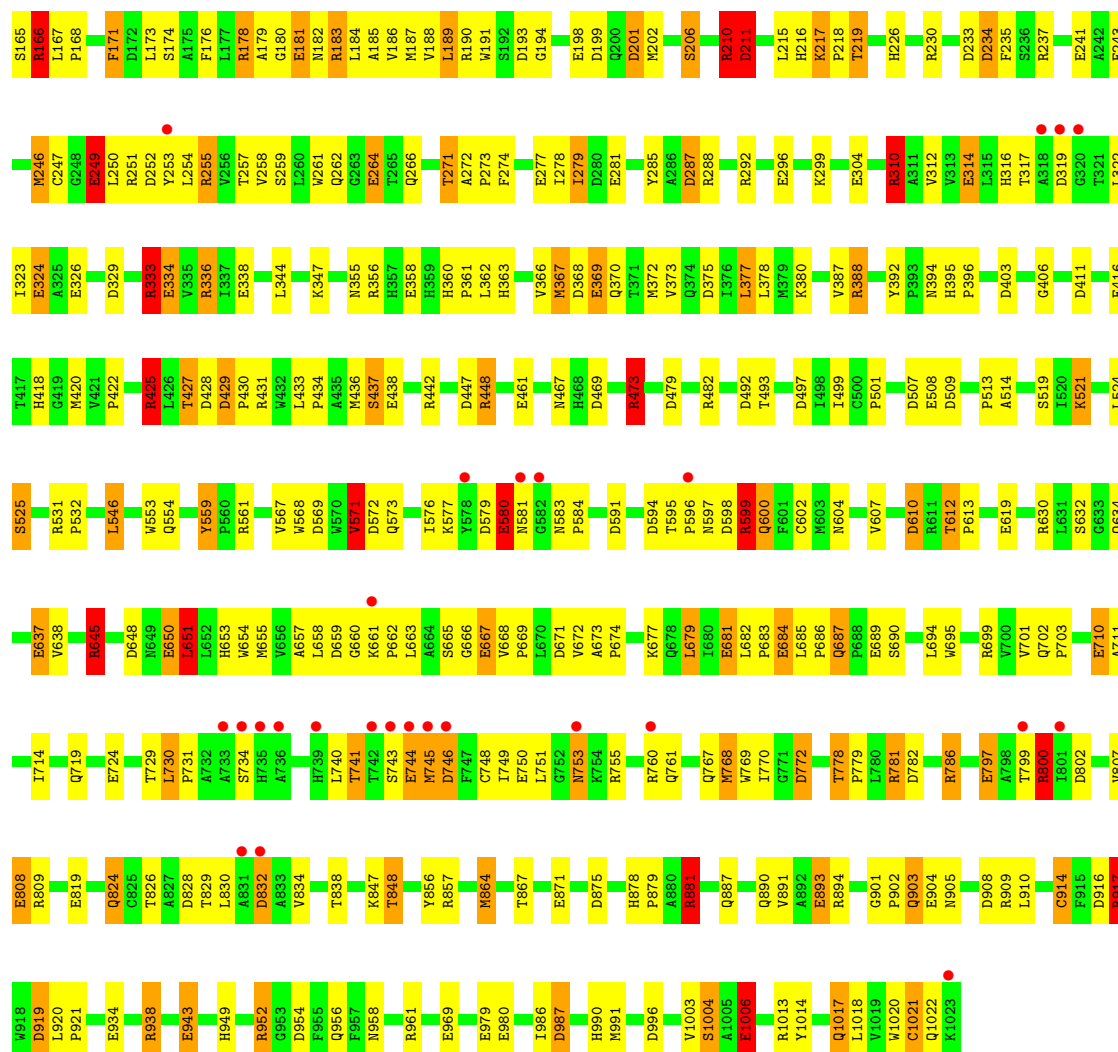
● Molecule 1: BETA-GALACTOSIDASE



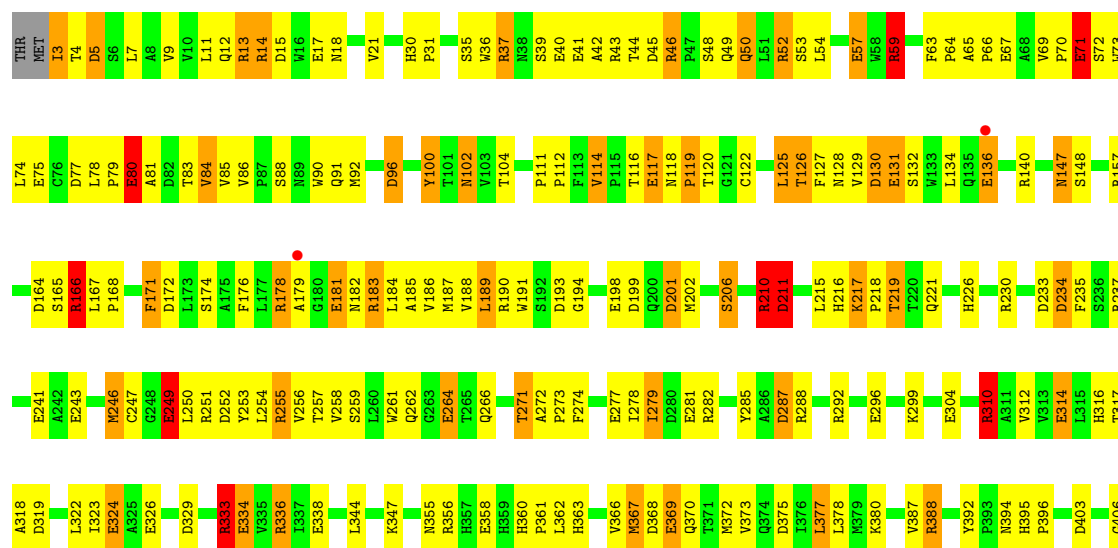
● Molecule 1: BETA-GALACTOSIDASE



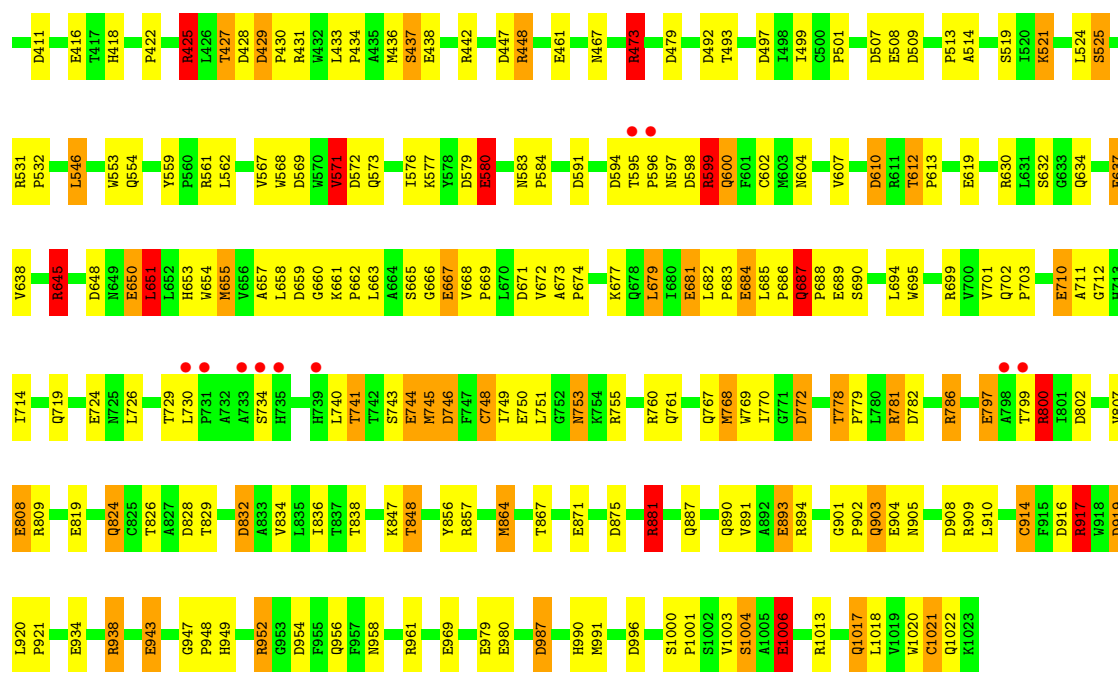




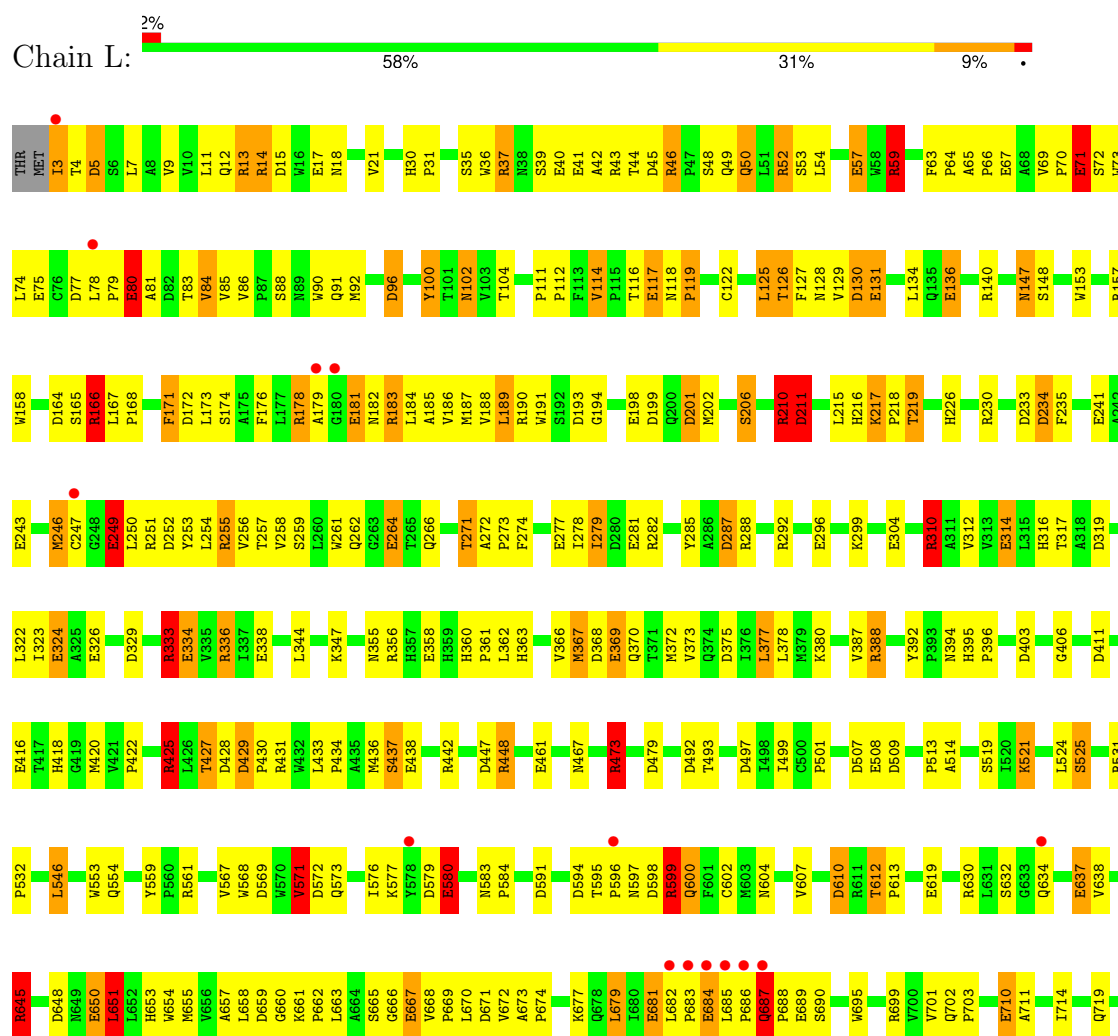
• Molecule 1: BETA-GALACTOSIDASE

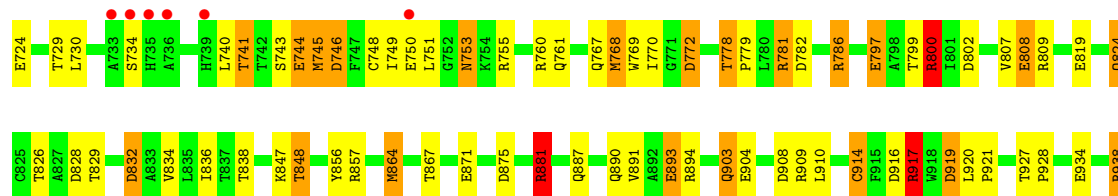




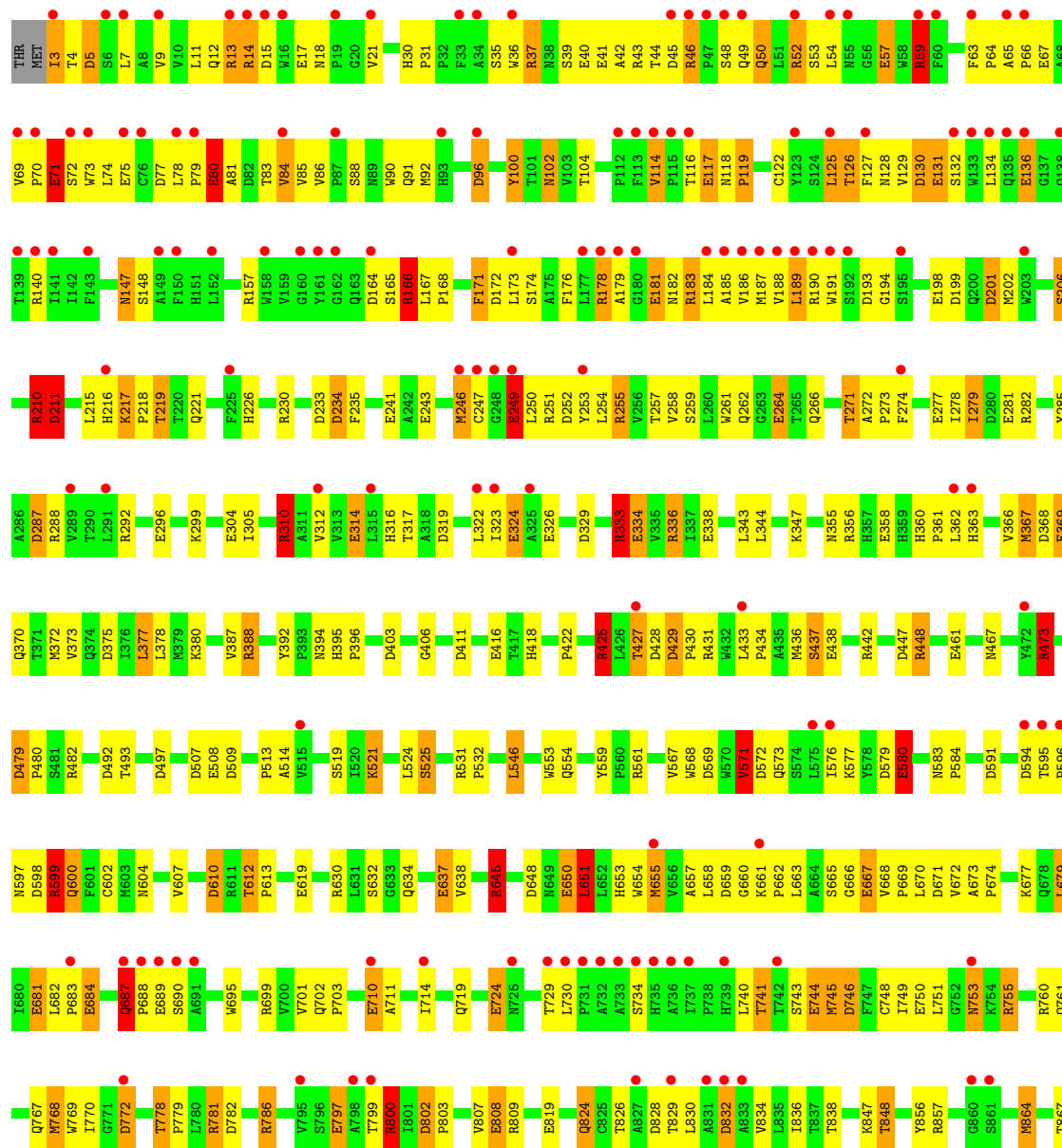


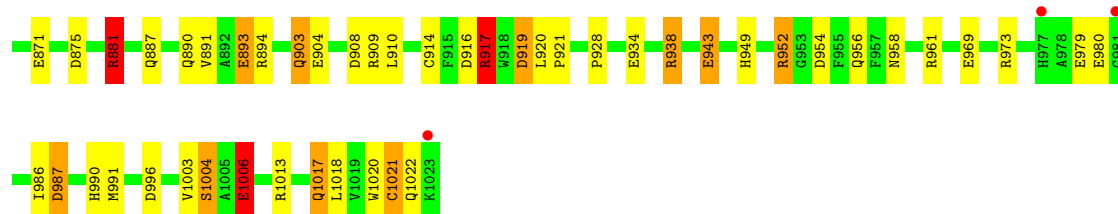
• Molecule 1: BETA-GALACTOSIDASE



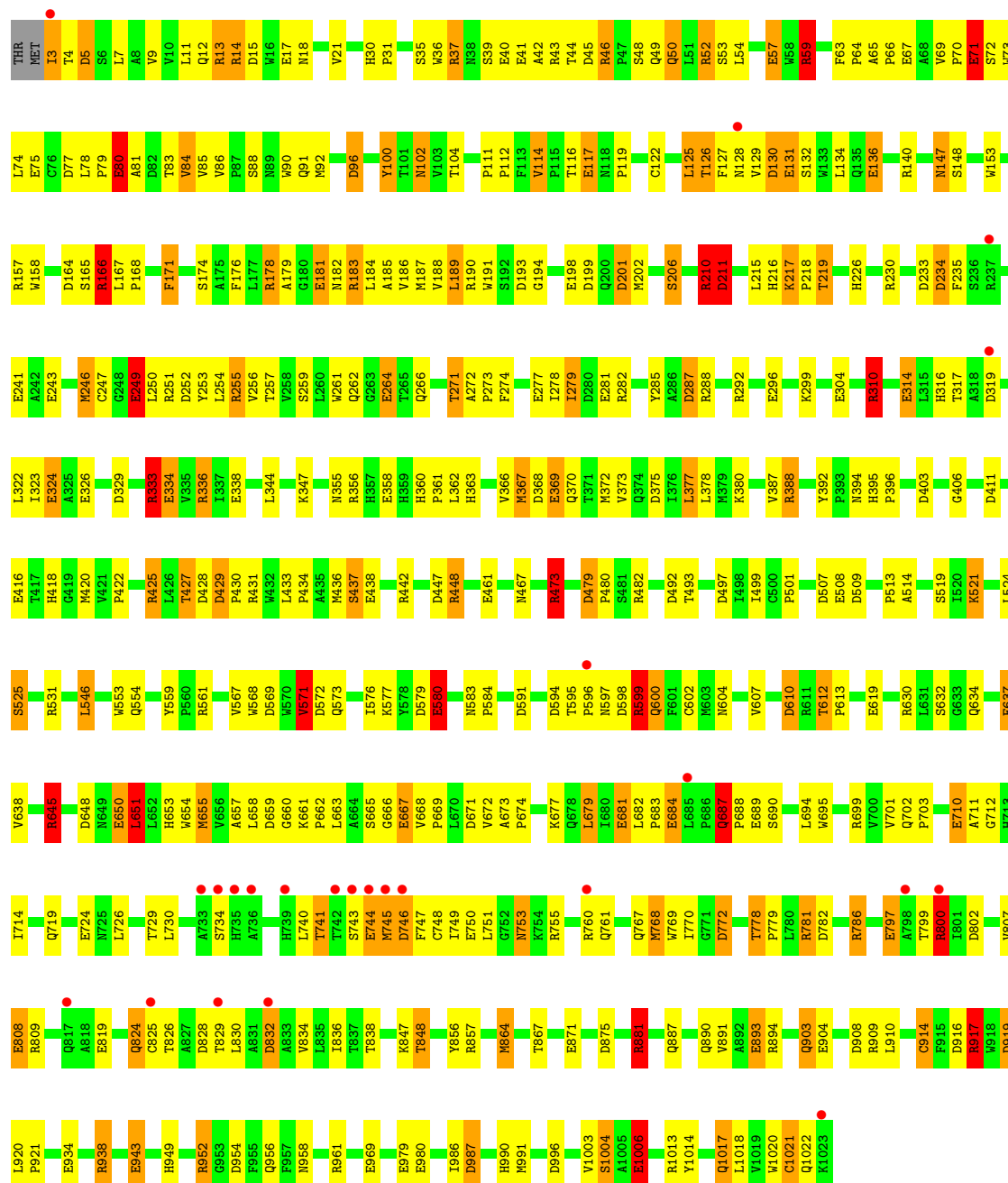


• Molecule 1: BETA-GALACTOSIDASE

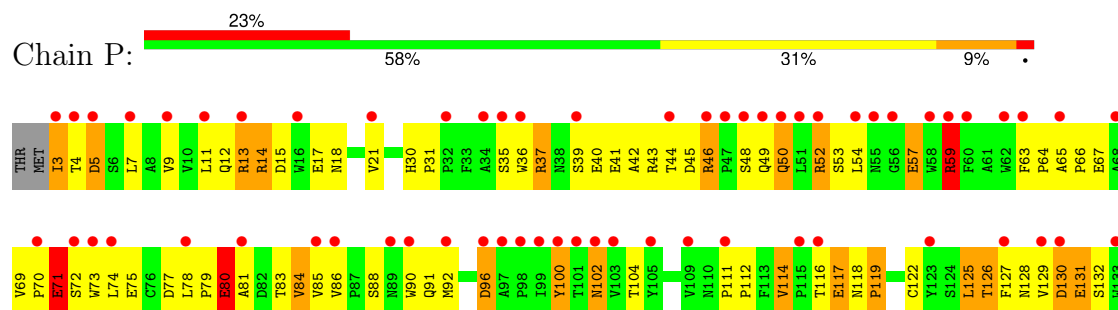


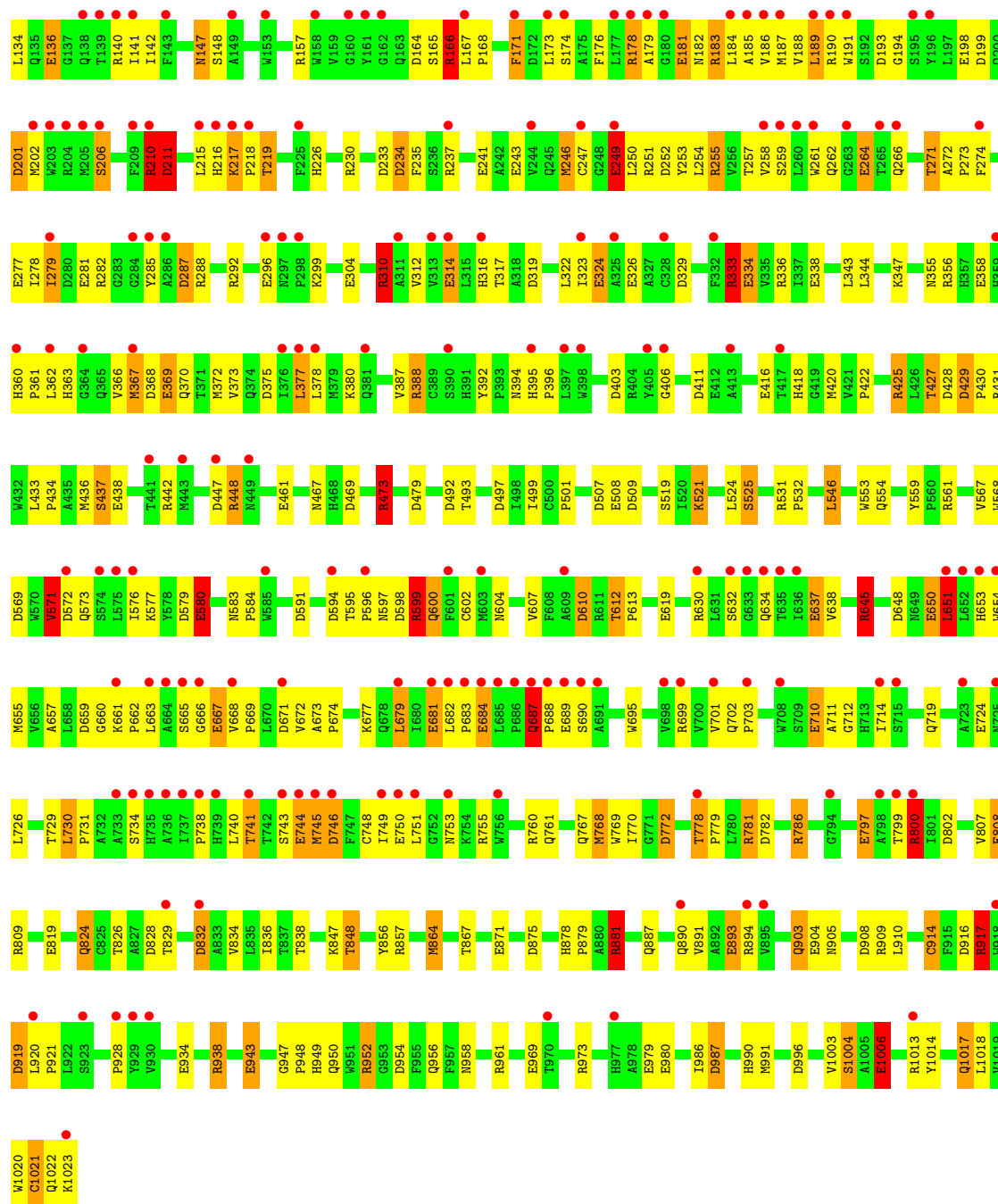


• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 200.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.0 ((Not available)-2.50) 72.7 (200.00-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.199 , 0.207 0.184 , 0.191	Depositor DCC
$R_{free}$ test set	1516 reflections (0.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 100.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	138704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: MG, CME

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	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	B	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	C	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	D	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	E	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	F	1.23	55/8472 (0.6%)	1.69	186/11553 (1.6%)
1	G	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	H	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	I	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	J	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	K	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	L	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	M	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	N	1.23	56/8472 (0.7%)	1.69	187/11553 (1.6%)
1	O	1.23	57/8472 (0.7%)	1.69	188/11553 (1.6%)
1	P	1.23	56/8472 (0.7%)	1.69	187/11553 (1.6%)
All	All	1.23	896/135552 (0.7%)	1.69	3010/184848 (1.6%)

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	2	0
1	B	2	0
1	C	2	0
1	D	2	0
1	E	2	0
1	F	2	0
1	G	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	2	0
1	I	2	0
1	J	2	0
1	K	2	0
1	L	2	0
1	M	2	0
1	N	2	0
1	O	2	0
1	P	2	0
All	All	32	0

The worst 5 of 896 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	GLU	CD-OE2	12.04	1.38	1.25
1	O	249	GLU	CD-OE2	12.03	1.38	1.25
1	H	249	GLU	CD-OE2	12.01	1.38	1.25
1	J	249	GLU	CD-OE2	12.01	1.38	1.25
1	P	249	GLU	CD-OE2	12.01	1.38	1.25

The worst 5 of 3010 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	210	ARG	NE-CZ-NH1	18.08	129.34	120.30
1	L	210	ARG	NE-CZ-NH1	18.07	129.34	120.30
1	J	210	ARG	NE-CZ-NH1	18.07	129.33	120.30
1	M	210	ARG	NE-CZ-NH1	18.03	129.31	120.30
1	G	210	ARG	NE-CZ-NH1	18.01	129.30	120.30

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	249	GLU	CA
1	B	166	ARG	CA
1	B	249	GLU	CA
1	C	166	ARG	CA

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	8232	0	7817	270	3
1	B	8232	0	7817	267	4
1	C	8232	0	7817	262	1
1	D	8232	0	7817	275	0
1	E	8232	0	7817	266	0
1	F	8232	0	7817	269	0
1	G	8232	0	7817	267	0
1	H	8232	0	7817	261	0
1	I	8232	0	7817	269	1
1	J	8232	0	7817	274	0
1	K	8232	0	7817	277	0
1	L	8232	0	7817	264	0
1	M	8232	0	7817	271	0
1	N	8232	0	7817	269	0
1	O	8232	0	7817	271	0
1	P	8232	0	7817	269	1
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	2	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	434	0	0	13	0
3	B	436	0	0	13	0
3	C	433	0	0	13	0
3	D	437	0	0	13	0
3	E	435	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	436	0	0	13	0
3	G	434	0	0	13	0
3	H	435	0	0	13	0
3	I	434	0	0	13	0
3	J	436	0	0	13	0
3	K	435	0	0	13	0
3	L	435	0	0	13	0
3	M	434	0	0	13	0
3	N	436	0	0	13	0
3	O	433	0	0	13	0
3	P	437	0	0	13	0
All	All	138704	0	125072	4201	5

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 16.

The worst 5 of 4201 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:L:427:THR:HA	1:L:436:MET:HE1	1.43	1.01
1:E:427:THR:HA	1:E:436:MET:HE1	1.41	1.00
1:M:427:THR:HA	1:M:436:MET:HE1	1.43	1.00
1:J:427:THR:HA	1:J:436:MET:HE1	1.44	0.99
1:C:427:THR:HA	1:C:436:MET:HE1	1.45	0.98

All (5) 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:CB[2_555]	1.77	0.43
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.85	0.35
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	2.10	0.10
1:B:739:HIS:NE2	1:P:738:PRO:O[1_354]	2.10	0.10
1:C:739:HIS:ND1	1:I:734:SER:O[1_655]	2.15	0.05

## 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	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	B	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	C	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	D	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	E	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	F	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	G	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	H	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	I	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	J	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	K	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	L	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	M	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	N	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	O	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
1	P	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	37	56
All	All	16336/16368 (100%)	15616 (96%)	672 (4%)	48 (0%)	37	56

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	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	B	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	C	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	D	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	E	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	F	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	G	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	H	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	I	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	J	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	K	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	L	875/872 (100%)	777 (89%)	98 (11%)	5	10
1	M	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	N	875/872 (100%)	777 (89%)	98 (11%)	5	10
1	O	875/872 (100%)	776 (89%)	99 (11%)	4	9
1	P	875/872 (100%)	776 (89%)	99 (11%)	4	9
All	All	14000/13952 (100%)	12418 (89%)	1582 (11%)	4	9

5 of 1582 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	262	GLN
1	L	580	GLU
1	J	632	SER
1	J	259	SER
1	K	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1017	GLN
1	P	128	ASN
1	J	949	HIS
1	O	1017	GLN
1	N	739	HIS

### 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	D	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	B	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	L	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	N	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	M	914	1	8,9,10	0.86	0	6,9,11	1.72	1 (16%)
1	CME	H	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	E	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	D	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	O	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	J	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	G	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	O	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	M	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	H	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	F	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	P	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CME	I	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	L	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	F	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	O	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.38	1 (16%)
1	CME	C	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	N	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	H	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	I	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	F	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	K	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	K	1021	1	8,9,10	1.29	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	A	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	C	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	B	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	K	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	E	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	G	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	M	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	P	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	D	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	L	914	1	8,9,10	0.85	0	6,9,11	1.73	1 (16%)
1	CME	P	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	J	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	C	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	B	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	N	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	E	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	I	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	A	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	J	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	A	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	G	914	1	8,9,10	0.84	0	6,9,11	1.72	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	D	1021	1	-	4/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-
1	CME	L	748	1	-	3/5/8/10	-
1	CME	N	914	1	-	3/5/8/10	-
1	CME	M	914	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	E	748	1	-	3/5/8/10	-
1	CME	D	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	3/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	G	1021	1	-	4/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	M	748	1	-	3/5/8/10	-
1	CME	H	1021	1	-	4/5/8/10	-
1	CME	F	914	1	-	3/5/8/10	-
1	CME	P	1021	1	-	4/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	L	1021	1	-	4/5/8/10	-
1	CME	F	748	1	-	3/5/8/10	-
1	CME	O	1021	1	-	4/5/8/10	-
1	CME	C	748	1	-	3/5/8/10	-
1	CME	N	748	1	-	3/5/8/10	-
1	CME	H	748	1	-	3/5/8/10	-
1	CME	I	1021	1	-	4/5/8/10	-
1	CME	F	1021	1	-	4/5/8/10	-
1	CME	K	748	1	-	3/5/8/10	-
1	CME	K	1021	1	-	4/5/8/10	-
1	CME	A	1021	1	-	4/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	B	748	1	-	3/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-
1	CME	E	914	1	-	3/5/8/10	-
1	CME	G	748	1	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	M	1021	1	-	4/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	D	748	1	-	3/5/8/10	-
1	CME	L	914	1	-	3/5/8/10	-
1	CME	P	748	1	-	3/5/8/10	-
1	CME	J	748	1	-	3/5/8/10	-
1	CME	C	1021	1	-	4/5/8/10	-
1	CME	B	1021	1	-	4/5/8/10	-
1	CME	N	1021	1	-	4/5/8/10	-
1	CME	E	1021	1	-	4/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-
1	CME	A	914	1	-	3/5/8/10	-
1	CME	J	1021	1	-	4/5/8/10	-
1	CME	A	748	1	-	3/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	748	CME	CA-N	-2.50	1.41	1.48
1	H	748	CME	CA-N	-2.50	1.41	1.48
1	K	748	CME	CA-N	-2.50	1.41	1.48
1	F	748	CME	CA-N	-2.49	1.41	1.48
1	G	748	CME	CA-N	-2.49	1.41	1.48

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1021	CME	CB-SG-SD	-8.04	83.06	103.86
1	K	1021	CME	CB-SG-SD	-8.03	83.07	103.86
1	P	1021	CME	CB-SG-SD	-8.03	83.08	103.86
1	N	1021	CME	CB-SG-SD	-8.03	83.09	103.86
1	I	1021	CME	CB-SG-SD	-8.02	83.10	103.86

There are no chirality outliers.

5 of 160 torsion outliers are listed below:



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

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1021	CME	3	0
1	B	914	CME	1	0
1	N	914	CME	1	0
1	H	914	CME	1	0
1	D	914	CME	1	0
1	J	914	CME	1	0
1	G	1021	CME	3	0
1	O	914	CME	1	0
1	H	1021	CME	3	0
1	P	1021	CME	3	0
1	I	914	CME	1	0
1	L	1021	CME	3	0
1	O	1021	CME	3	0
1	I	1021	CME	3	0
1	F	1021	CME	3	0
1	K	748	CME	1	0
1	K	1021	CME	3	0
1	A	1021	CME	3	0
1	C	914	CME	1	0
1	K	914	CME	1	0
1	M	1021	CME	3	0
1	P	914	CME	1	0
1	D	748	CME	1	0
1	L	914	CME	1	0
1	C	1021	CME	3	0
1	B	1021	CME	3	0
1	N	1021	CME	3	0
1	E	1021	CME	3	0
1	A	914	CME	1	0
1	J	1021	CME	3	0
1	A	748	CME	1	0
1	G	914	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	1018/1023 (99%)	-0.24	34 (3%)	49	46	3, 21, 66, 100	6 (0%)
1	B	1018/1023 (99%)	-0.22	36 (3%)	47	44	3, 21, 66, 100	6 (0%)
1	C	1018/1023 (99%)	-0.19	32 (3%)	51	48	2, 19, 63, 98	6 (0%)
1	D	1018/1023 (99%)	-0.06	36 (3%)	47	44	5, 23, 67, 100	6 (0%)
1	E	1018/1023 (99%)	0.37	46 (4%)	39	36	15, 33, 74, 100	6 (0%)
1	F	1018/1023 (99%)	-0.29	26 (2%)	57	54	3, 21, 66, 100	6 (0%)
1	G	1018/1023 (99%)	-0.19	21 (2%)	63	60	7, 25, 68, 100	6 (0%)
1	H	1018/1023 (99%)	0.15	34 (3%)	49	46	14, 32, 73, 100	6 (0%)
1	I	1018/1023 (99%)	-0.04	22 (2%)	62	59	10, 28, 70, 100	6 (0%)
1	J	1018/1023 (99%)	-0.17	29 (2%)	55	51	8, 26, 69, 100	6 (0%)
1	K	1018/1023 (99%)	-0.01	12 (1%)	76	73	17, 35, 76, 100	6 (0%)
1	L	1018/1023 (99%)	0.10	22 (2%)	62	59	16, 34, 75, 100	6 (0%)
1	M	1018/1023 (99%)	0.99	143 (14%)	7	7	22, 40, 79, 100	6 (0%)
1	N	1018/1023 (99%)	-0.04	24 (2%)	59	56	11, 29, 71, 100	6 (0%)
1	O	1018/1023 (99%)	-0.06	22 (2%)	62	59	12, 30, 72, 100	6 (0%)
1	P	1018/1023 (99%)	1.40	234 (22%)	2	3	29, 47, 83, 100	6 (0%)
All	All	16288/16368 (99%)	0.09	773 (4%)	37	34	2, 30, 72, 100	96 (0%)

The worst 5 of 773 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.3
1	D	734	SER	7.3
1	A	581	ASN	7.0
1	B	582	GLY	6.4
1	P	684	GLU	6.1

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CME	P	748	10/11	0.83	0.17	44,54,100,100	0
1	CME	P	914	10/11	0.85	0.16	34,40,100,100	0
1	CME	C	748	10/11	0.88	0.16	16,26,97,97	0
1	CME	L	748	10/11	0.88	0.17	31,41,100,100	0
1	CME	H	748	10/11	0.89	0.15	29,39,100,100	0
1	CME	N	1021	10/11	0.90	0.14	9,33,100,100	0
1	CME	B	748	10/11	0.90	0.14	18,28,99,99	0
1	CME	M	1021	10/11	0.90	0.14	21,44,100,100	0
1	CME	P	1021	10/11	0.90	0.14	28,51,100,100	0
1	CME	F	1021	10/11	0.91	0.13	2,25,100,100	0
1	CME	I	1021	10/11	0.92	0.13	9,32,100,100	0
1	CME	J	1021	10/11	0.92	0.12	7,30,100,100	0
1	CME	O	1021	10/11	0.92	0.12	11,34,100,100	0
1	CME	K	748	10/11	0.92	0.13	32,42,100,100	0
1	CME	H	1021	10/11	0.92	0.13	13,36,100,100	0
1	CME	M	914	10/11	0.92	0.15	27,33,100,100	0
1	CME	L	1021	10/11	0.93	0.11	15,38,100,100	0
1	CME	E	1021	10/11	0.93	0.13	14,37,100,100	0
1	CME	C	1021	10/11	0.93	0.13	1,23,97,97	0
1	CME	J	748	10/11	0.93	0.11	23,33,100,100	0
1	CME	G	748	10/11	0.93	0.11	22,32,100,100	0
1	CME	G	1021	10/11	0.93	0.10	6,29,100,100	0
1	CME	K	1021	10/11	0.93	0.11	16,39,100,100	0
1	CME	D	748	10/11	0.93	0.15	21,30,100,100	0
1	CME	E	748	10/11	0.94	0.13	30,40,100,100	0
1	CME	A	1021	10/11	0.94	0.12	2,25,100,100	0
1	CME	O	748	10/11	0.94	0.13	27,37,100,100	0
1	CME	F	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	I	748	10/11	0.94	0.11	25,35,100,100	0
1	CME	A	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	B	1021	10/11	0.94	0.11	2,25,99,99	0
1	CME	O	914	10/11	0.95	0.10	17,23,100,100	0
1	CME	D	1021	10/11	0.95	0.13	4,27,100,100	0
1	CME	N	748	10/11	0.95	0.10	26,35,100,100	0
1	CME	M	748	10/11	0.95	0.11	37,47,100,100	0
1	CME	H	914	10/11	0.95	0.12	19,25,100,100	0
1	CME	K	914	10/11	0.96	0.10	22,28,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CME	G	914	10/11	0.96	0.10	12,18,100,100	0
1	CME	I	914	10/11	0.96	0.10	15,21,100,100	0
1	CME	L	914	10/11	0.96	0.10	21,27,100,100	0
1	CME	E	914	10/11	0.97	0.10	20,26,100,100	0
1	CME	A	914	10/11	0.97	0.10	8,14,100,100	0
1	CME	N	914	10/11	0.97	0.10	16,22,100,100	0
1	CME	J	914	10/11	0.97	0.10	13,19,100,100	0
1	CME	B	914	10/11	0.97	0.10	8,14,99,99	0
1	CME	C	914	10/11	0.98	0.09	6,12,97,97	0
1	CME	F	914	10/11	0.98	0.08	8,14,100,100	0
1	CME	D	914	10/11	0.98	0.09	10,16,100,100	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	3002	1/1	0.90	0.09	16,16,16,16	0
2	MG	M	3002	1/1	0.91	0.14	37,37,37,37	0
2	MG	P	3002	1/1	0.91	0.08	44,44,44,44	0
2	MG	P	3001	1/1	0.92	0.12	44,44,44,44	0
2	MG	E	3002	1/1	0.92	0.09	30,30,30,30	0
2	MG	M	3001	1/1	0.93	0.12	37,37,37,37	0
2	MG	L	3001	1/1	0.94	0.05	31,31,31,31	0
2	MG	I	3001	1/1	0.95	0.07	25,25,25,25	0
2	MG	I	3002	1/1	0.95	0.08	25,25,25,25	0
2	MG	B	3002	1/1	0.95	0.06	18,18,18,18	0
2	MG	L	3002	1/1	0.95	0.07	31,31,31,31	0
2	MG	D	3002	1/1	0.96	0.07	21,21,21,21	0
2	MG	H	3002	1/1	0.96	0.08	30,30,30,30	0
2	MG	K	3002	1/1	0.96	0.05	32,32,32,32	0
2	MG	A	3002	1/1	0.97	0.09	18,18,18,18	0
2	MG	J	3002	1/1	0.97	0.10	23,23,23,23	0
2	MG	F	3002	1/1	0.97	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	G	3002	1/1	0.98	0.05	22,22,22,22	0
2	MG	J	3001	1/1	0.98	0.07	23,23,23,23	0
2	MG	H	3001	1/1	0.98	0.03	29,29,29,29	0
2	MG	N	3001	1/1	0.98	0.04	26,26,26,26	0
2	MG	N	3002	1/1	0.98	0.09	26,26,26,26	0
2	MG	O	3002	1/1	0.98	0.08	27,27,27,27	0
2	MG	B	3001	1/1	0.98	0.03	18,18,18,18	0
2	MG	A	3001	1/1	0.98	0.10	18,18,18,18	0
2	MG	D	3001	1/1	0.99	0.03	20,20,20,20	0
2	MG	K	3001	1/1	0.99	0.08	32,32,32,32	0
2	MG	F	3001	1/1	0.99	0.03	18,18,18,18	0
2	MG	O	3001	1/1	0.99	0.03	27,27,27,27	0
2	MG	C	3001	1/1	0.99	0.03	16,16,16,16	0
2	MG	G	3001	1/1	0.99	0.03	22,22,22,22	0
2	MG	E	3001	1/1	0.99	0.07	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.