



wwPDB X-ray Structure Validation Summary Report

Sep 17, 2023 – 01:53 AM EDT

PDB ID : 4V45
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

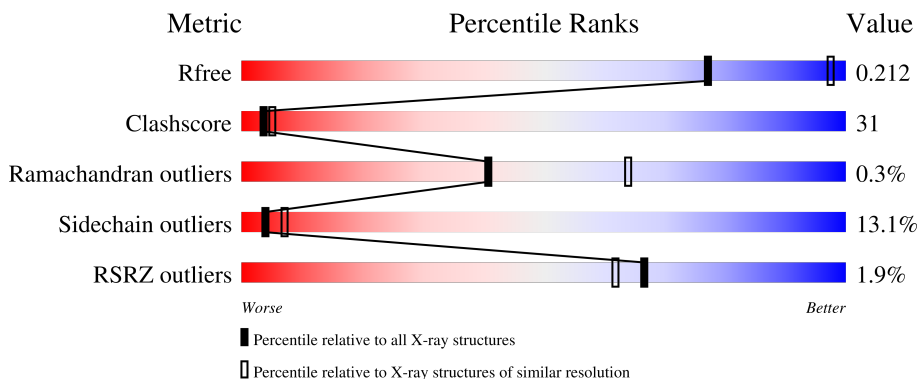
1 Overall quality at a glance

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.




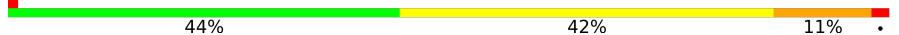

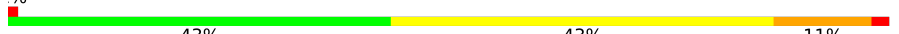
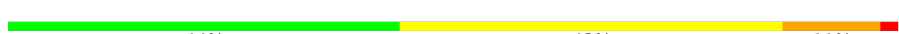

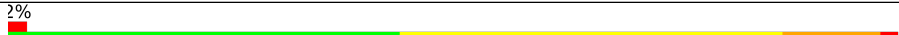
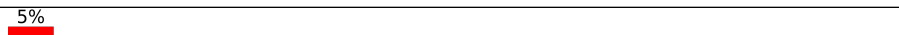
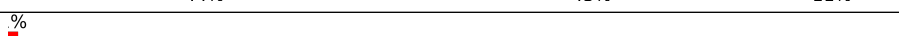
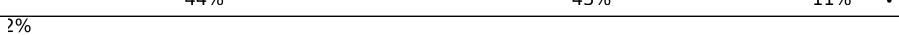
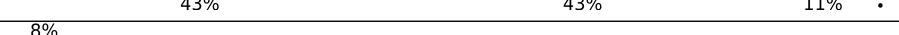
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	
1	B	1023	
1	C	1023	
1	D	1023	
1	E	1023	

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Mol	Chain	Length	Quality of chain
1	F	1023	 44% 43% 11% .
1	G	1023	 44% 42% 11% .
1	H	1023	 44% 43% 11% .
1	I	1023	 43% 43% 11% .
1	J	1023	 44% 43% 11% .
1	K	1023	 44% 43% 11% .
1	L	1023	 44% 43% 11% .
1	M	1023	 44% 43% 11% .
1	N	1023	 44% 43% 11% .
1	O	1023	 43% 43% 11% .
1	P	1023	 44% 43% 11% .

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	-	-	-

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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
			Total	C	N	O	S			
1	A	1021	8219	5196	1454	1528	41	0	2	0
1	B	1021	8219	5196	1454	1528	41	0	2	0
1	C	1021	8219	5196	1454	1528	41	0	2	0
1	D	1021	8219	5196	1454	1528	41	0	2	0
1	E	1021	8219	5196	1454	1528	41	0	2	0
1	F	1021	8219	5196	1454	1528	41	0	2	0
1	G	1021	8219	5196	1454	1528	41	0	2	0
1	H	1021	8219	5196	1454	1528	41	0	2	0
1	I	1021	8219	5196	1454	1528	41	0	2	0
1	J	1021	8219	5196	1454	1528	41	0	2	0
1	K	1021	8219	5196	1454	1528	41	0	2	0
1	L	1021	8219	5196	1454	1528	41	0	2	0
1	M	1021	8219	5196	1454	1528	41	0	2	0
1	N	1021	8219	5196	1454	1528	41	0	2	0
1	O	1021	8219	5196	1454	1528	41	0	2	0
1	P	1021	8219	5196	1454	1528	41	0	2	0

There are 48 discrepancies between the modelled and reference sequences:

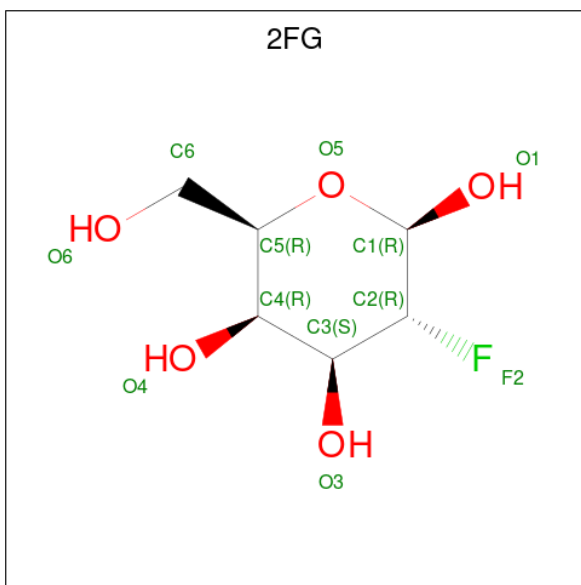
Chain	Residue	Modelled	Actual	Comment	Reference
A	748	CME	CYS	modified residue	UNP P00722
A	914	CME	CYS	modified residue	UNP P00722
A	1021	CME	CYS	modified residue	UNP P00722
B	748	CME	CYS	modified residue	UNP P00722
B	914	CME	CYS	modified residue	UNP P00722
B	1021	CME	CYS	modified residue	UNP P00722
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 2-deoxy-2-fluoro-beta-D-galactopyranose (three-letter code: 2FG) (formula: C₆H₁₁FO₅).



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		

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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 (three-letter code: 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		

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

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

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

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

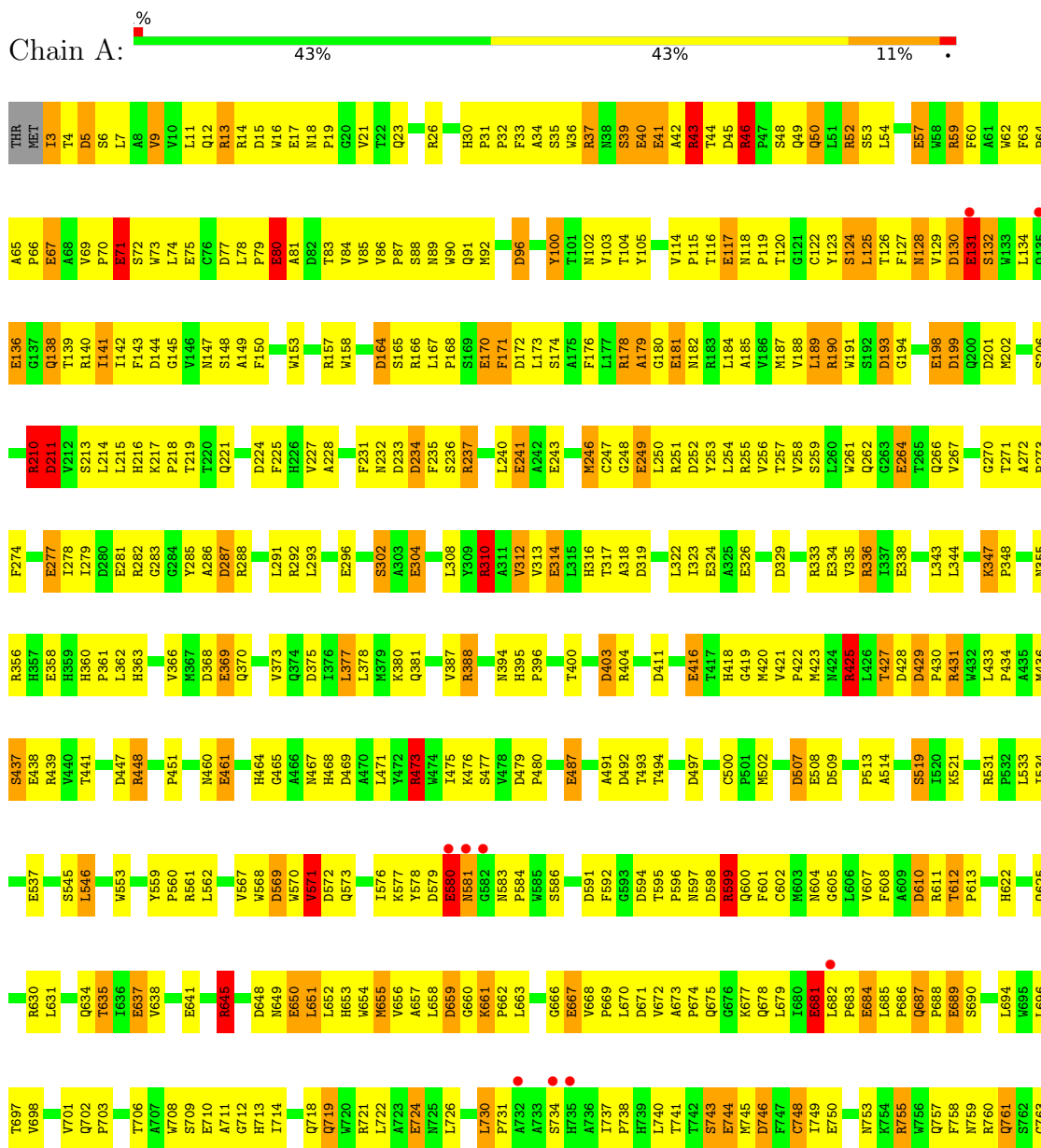
- Molecule 5 is water.

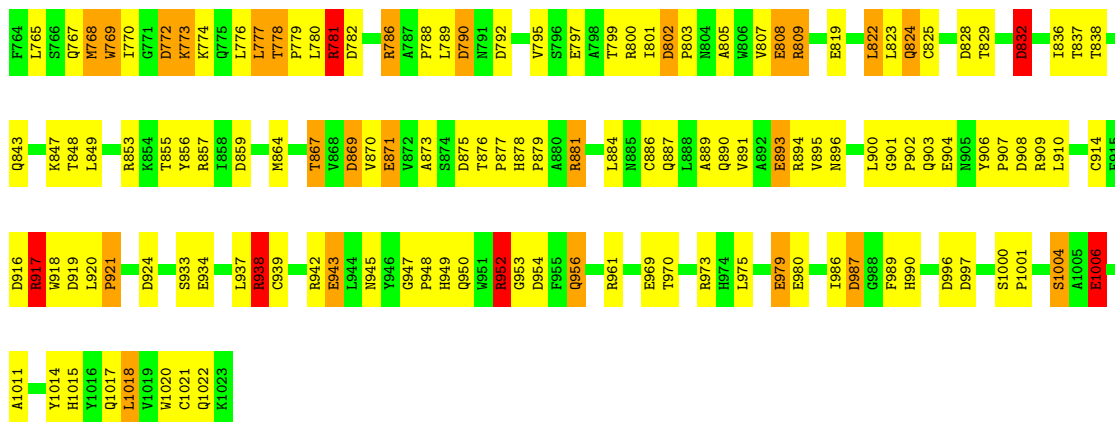
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total 140	O 140	0	0
5	B	140	Total 140	O 140	0	0
5	C	140	Total 140	O 140	0	0
5	D	140	Total 140	O 140	0	0
5	E	139	Total 139	O 139	0	0
5	F	140	Total 140	O 140	0	0
5	G	140	Total 140	O 140	0	0
5	H	141	Total 141	O 141	0	0
5	I	140	Total 140	O 140	0	0
5	J	140	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 [\(i\)](#)

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

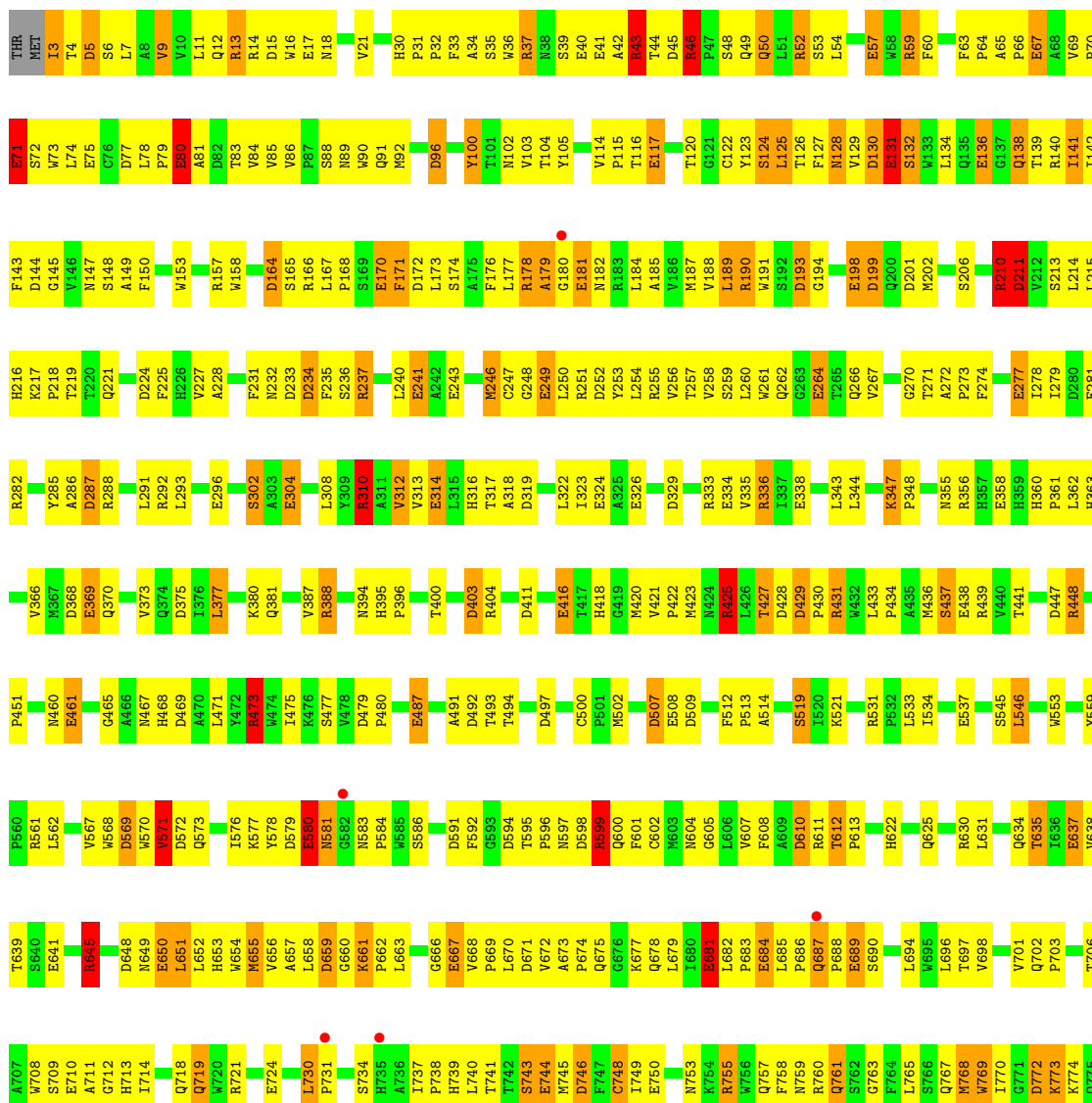
- Molecule 1: Beta-Galactosidase

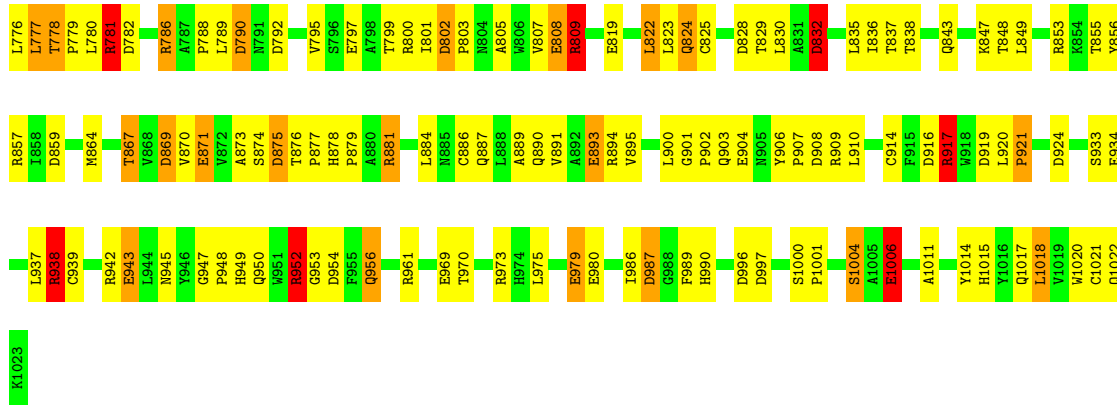




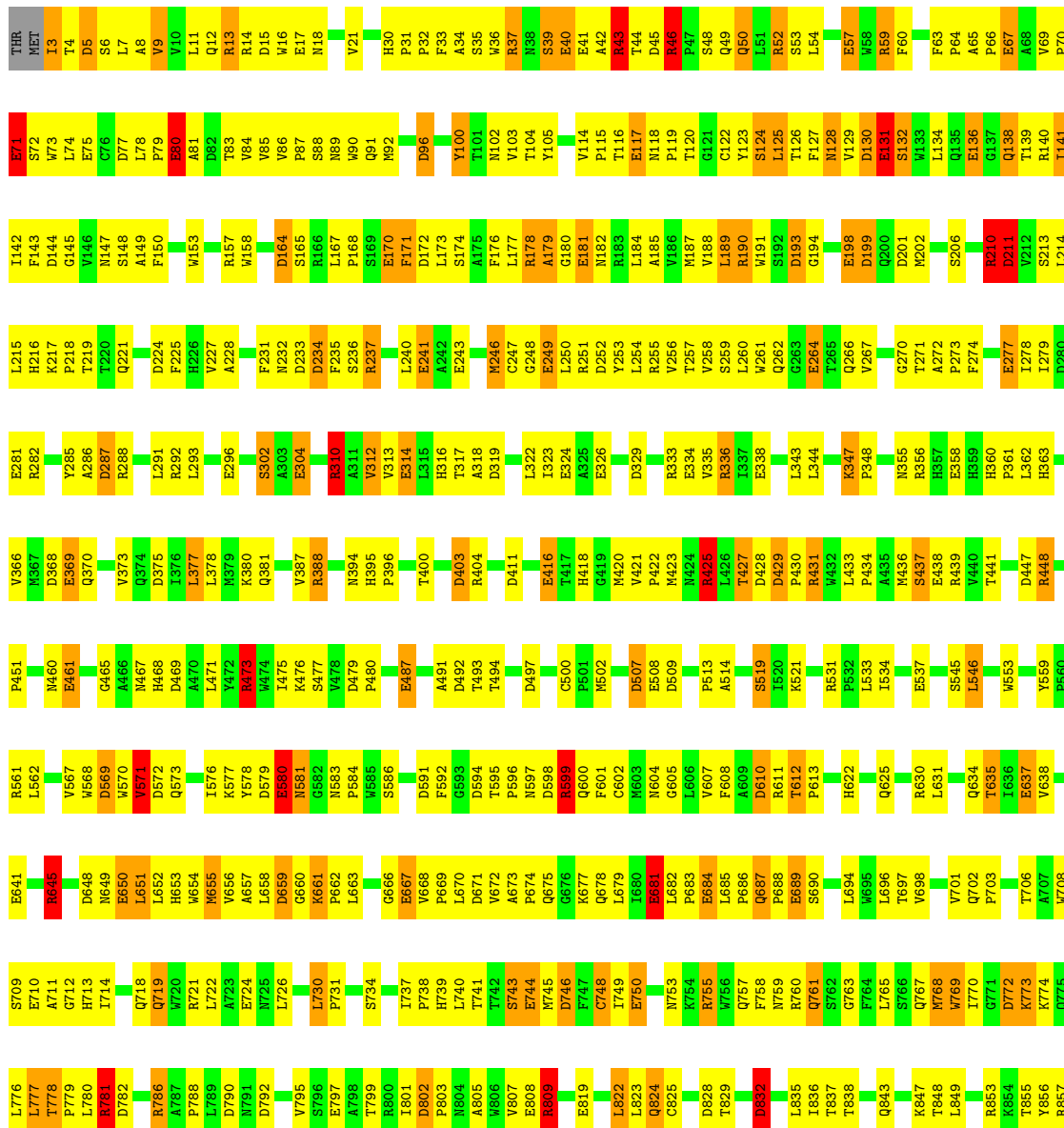
● Molecule 1: Beta-Galactosidase

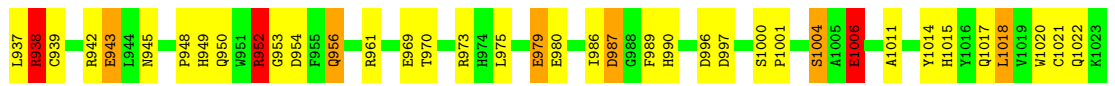
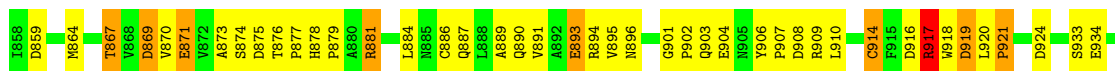
Chain B: 44% 43% 11%



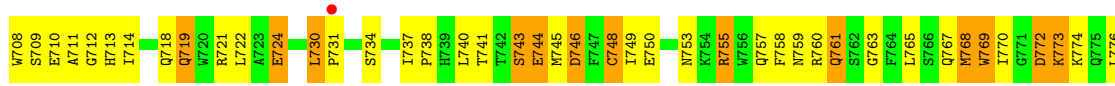
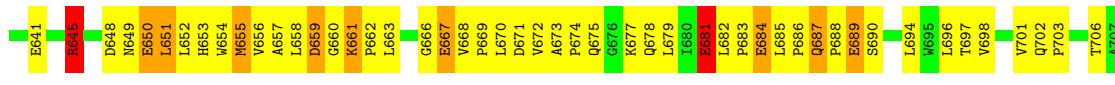
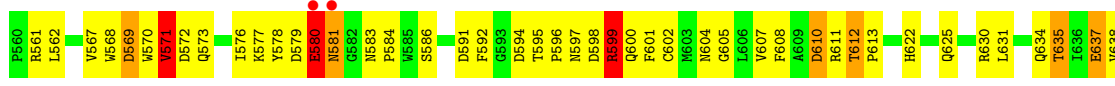
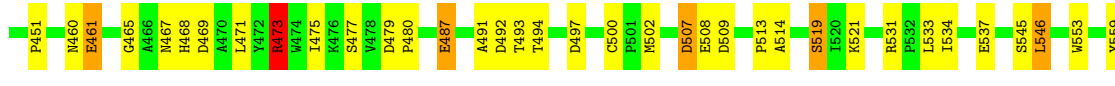
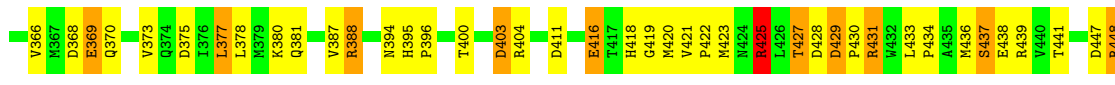
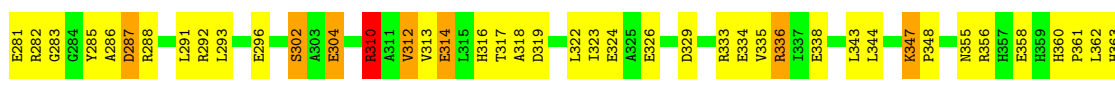
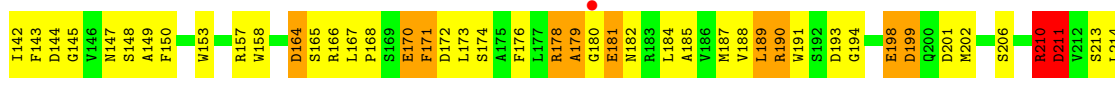
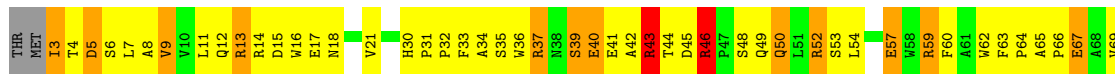


• Molecule 1: Beta-Galactosidase



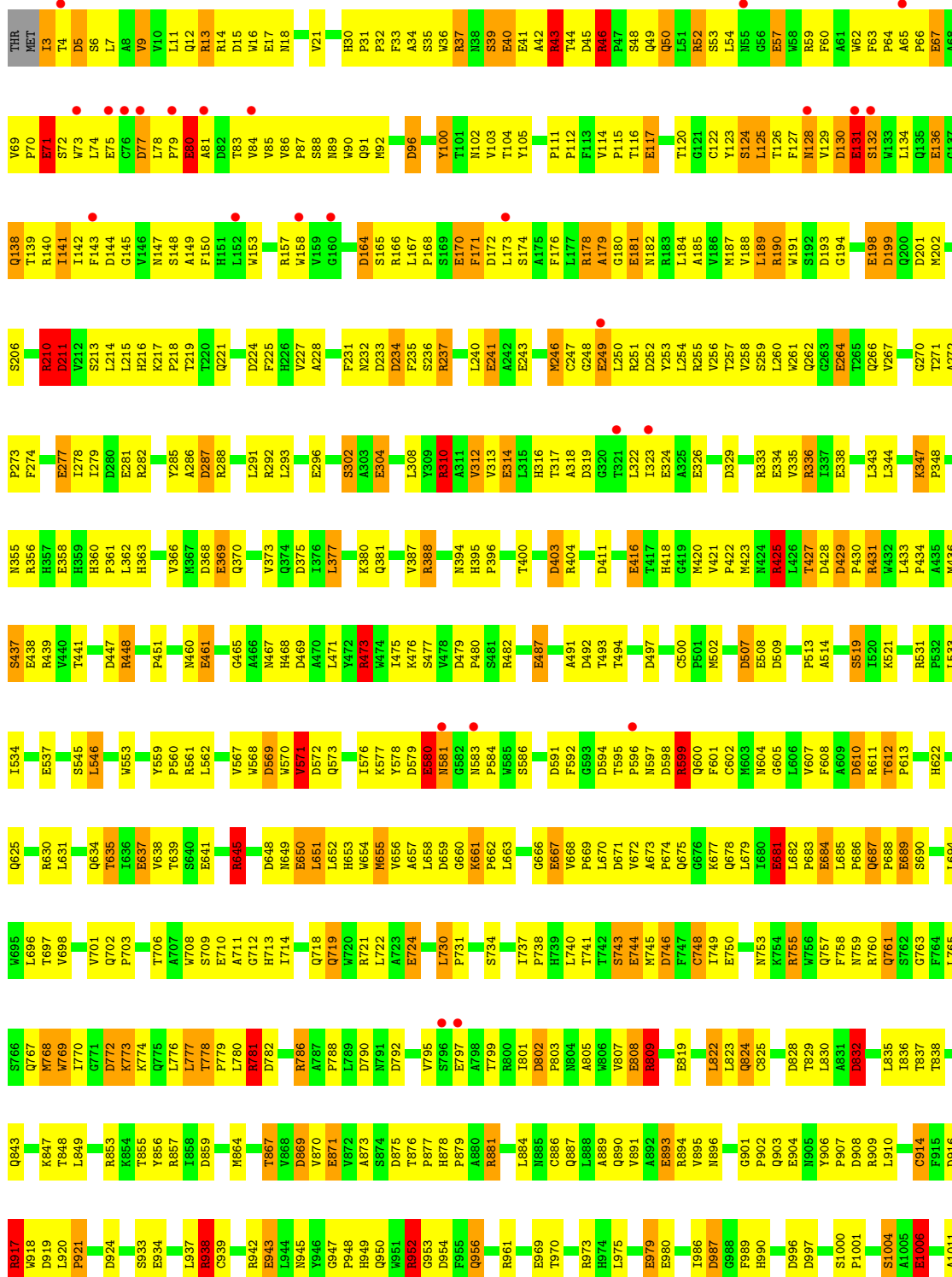


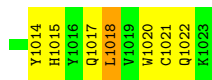
● Molecule 1: Beta-Galactosidase



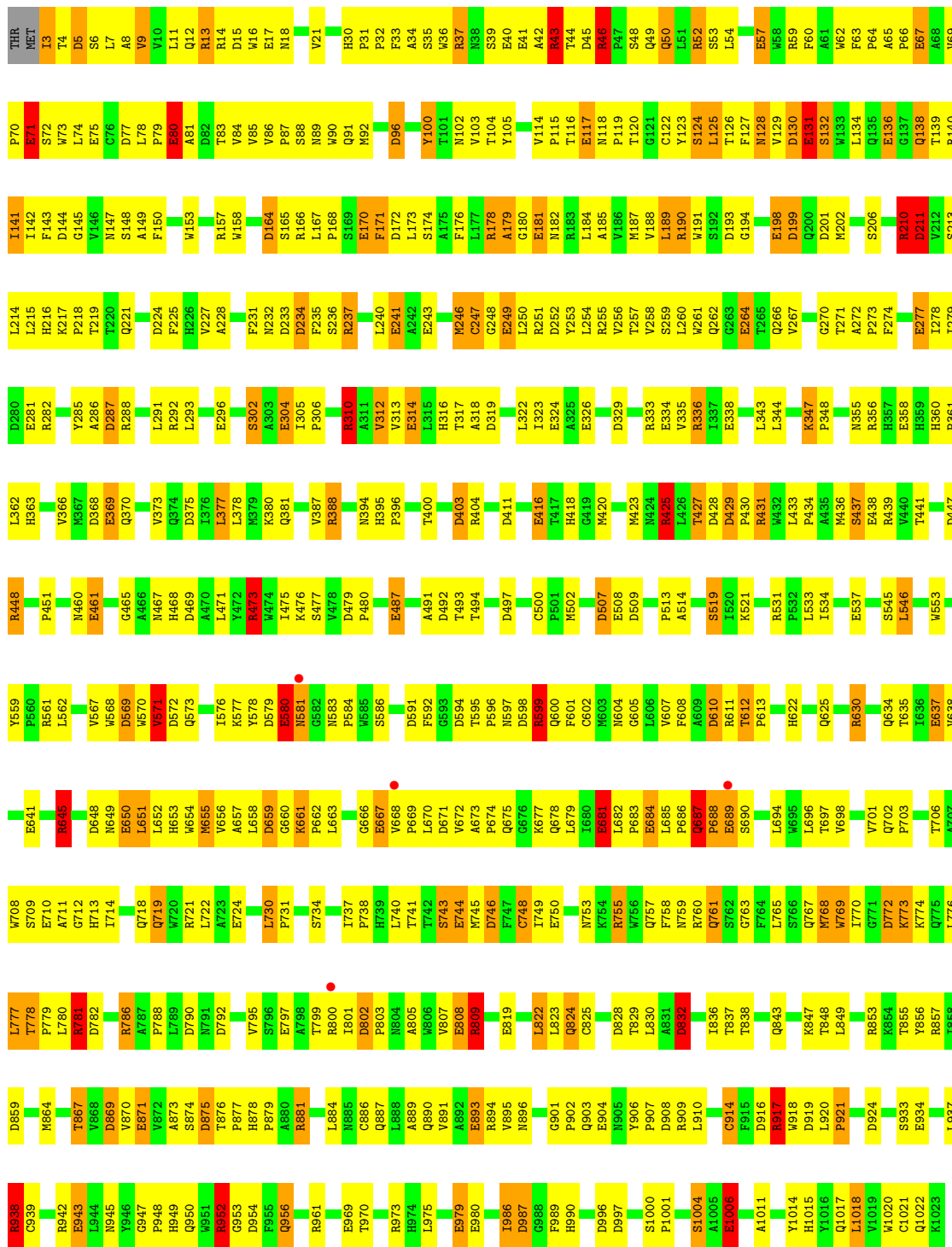


• Molecule 1: Beta-Galactosidase

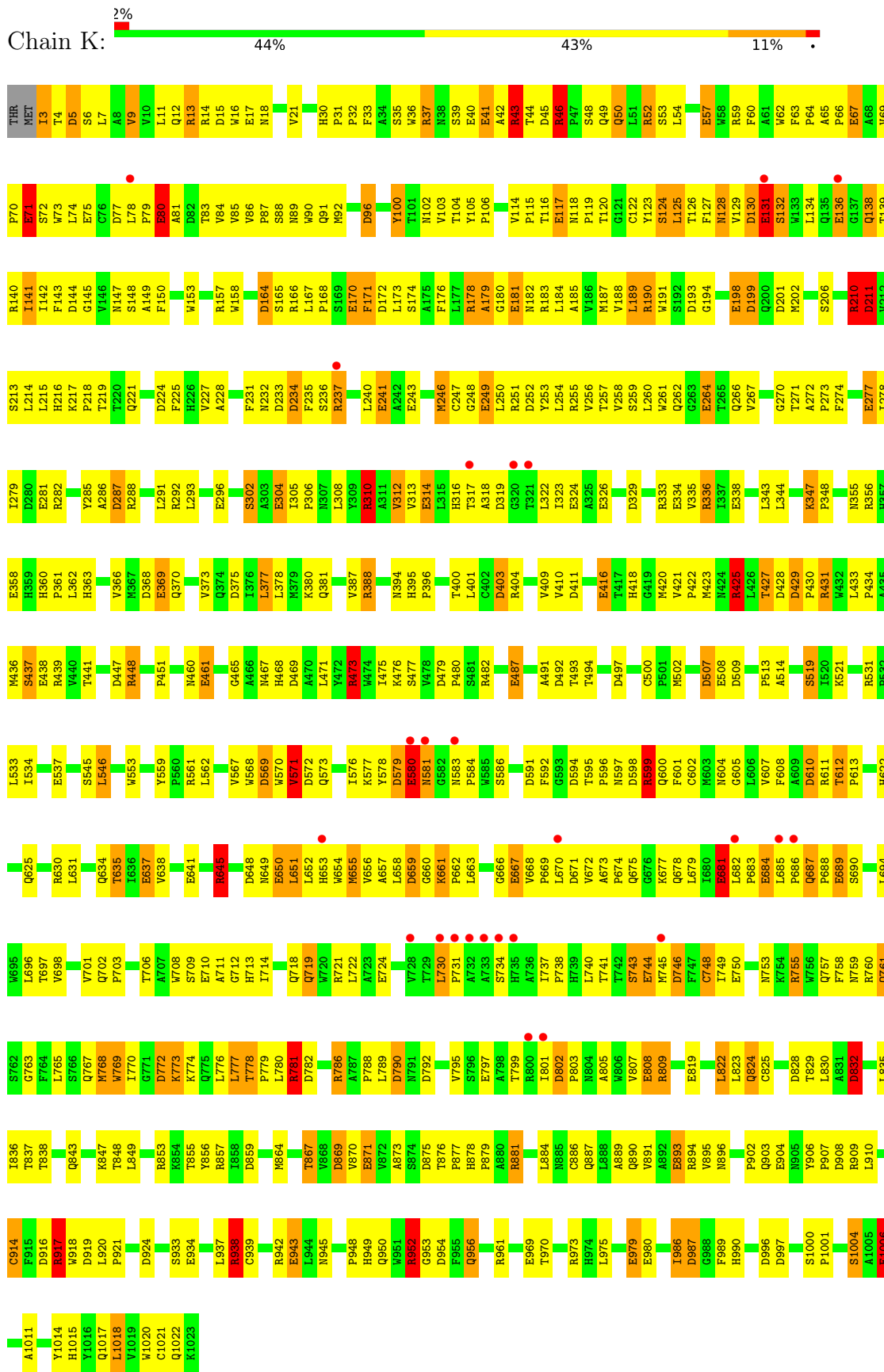




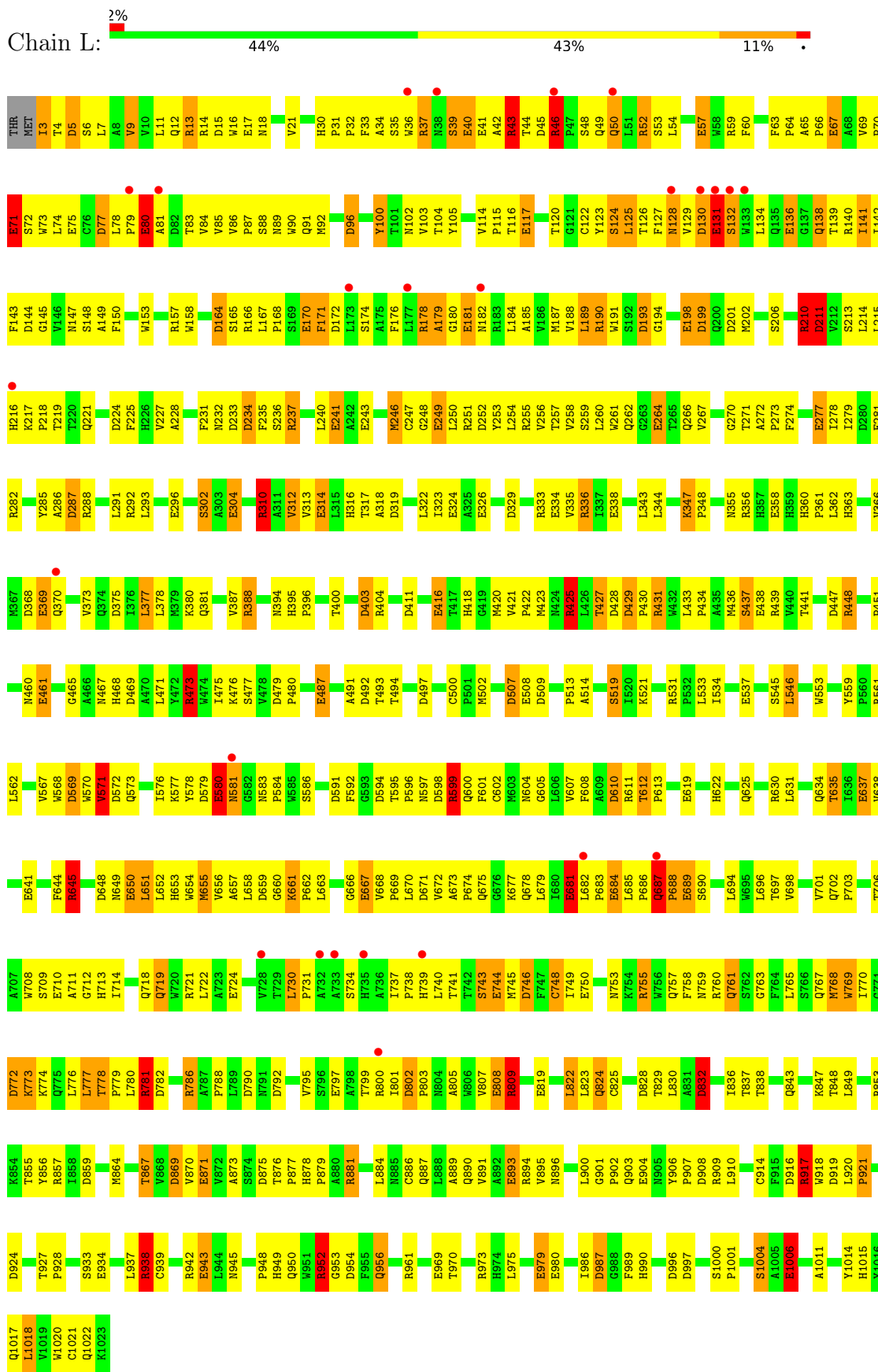
• Molecule 1: Beta-Galactosidase



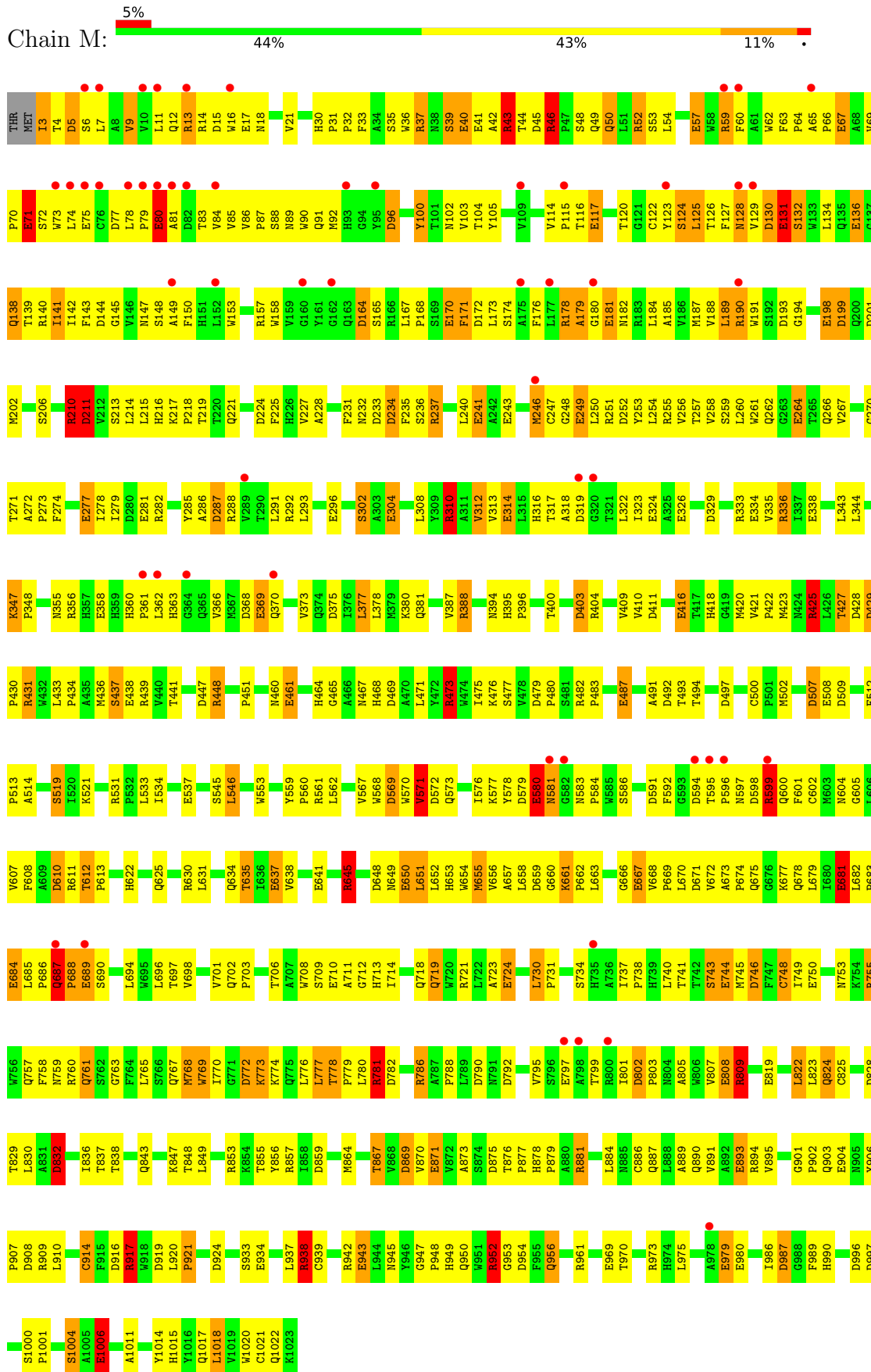
• Molecule 1: Beta-Galactosidase

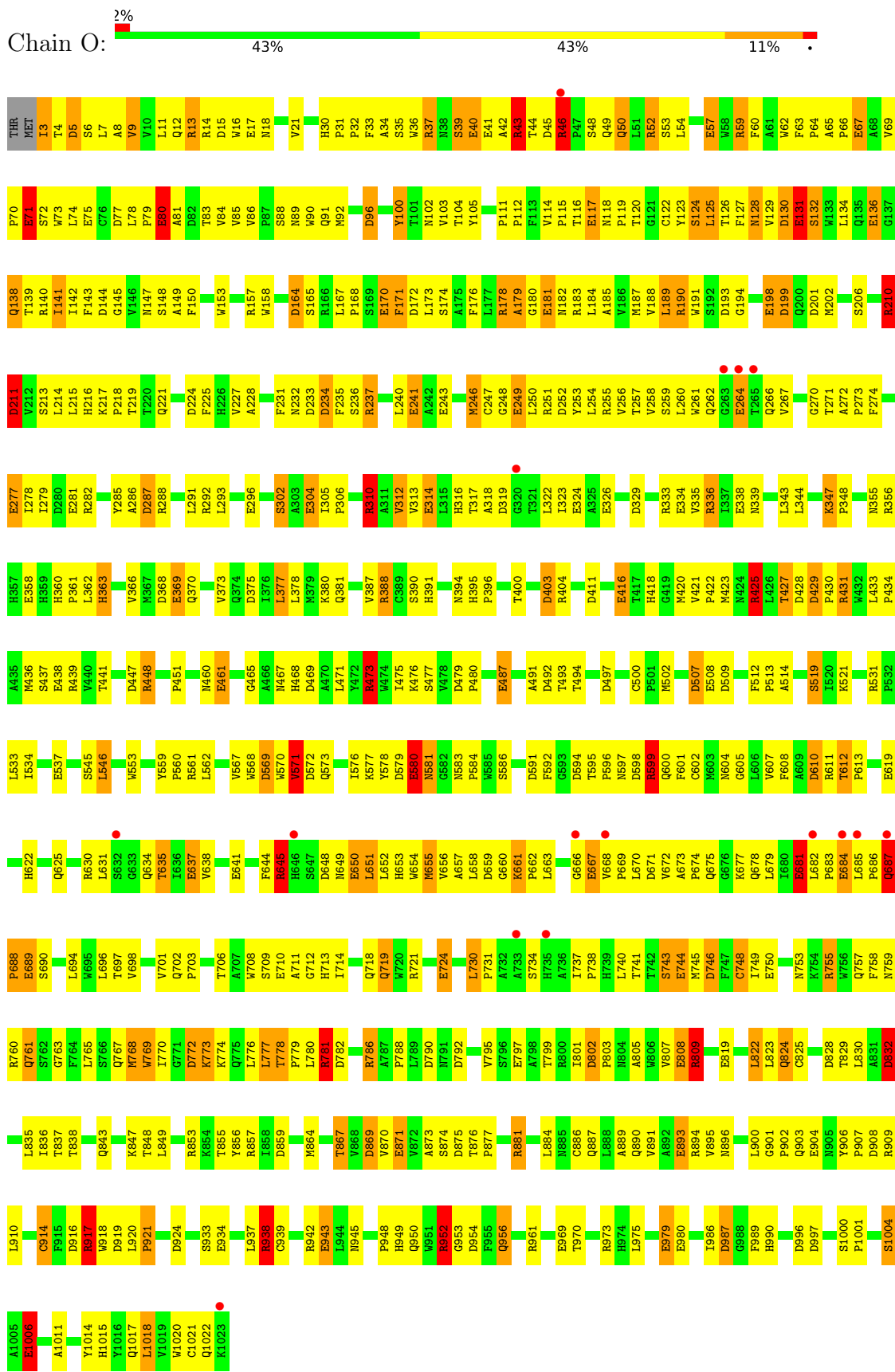


• Molecule 1: Beta-Galactosidase



• 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, α , β , γ	107.50Å 207.20Å 510.20Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	68.50 – 2.60 68.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	70.0 (68.50-2.60) 66.9 (68.52-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.51Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.230 , (Not available) 0.211 , 0.212	Depositor DCC
R_{free} test set	2386 reflections (0.46%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2FG, CME, NA

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	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	B	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	C	1.20	53/8439 (0.6%)	1.62	159/11510 (1.4%)
1	D	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	E	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	F	1.20	54/8439 (0.6%)	1.62	156/11510 (1.4%)
1	G	1.20	55/8439 (0.7%)	1.62	159/11510 (1.4%)
1	H	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	I	1.20	54/8439 (0.6%)	1.62	161/11510 (1.4%)
1	J	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	K	1.20	54/8439 (0.6%)	1.62	157/11510 (1.4%)
1	L	1.20	55/8439 (0.7%)	1.62	158/11510 (1.4%)
1	M	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	N	1.20	54/8439 (0.6%)	1.62	158/11510 (1.4%)
1	O	1.20	55/8439 (0.7%)	1.62	157/11510 (1.4%)
1	P	1.20	55/8439 (0.7%)	1.62	160/11510 (1.4%)
All	All	1.20	867/135024 (0.6%)	1.62	2531/184160 (1.4%)

The worst 5 of 867 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	GLU	CD-OE2	9.75	1.36	1.25
1	H	131	GLU	CD-OE2	9.74	1.36	1.25
1	C	131	GLU	CD-OE2	9.73	1.36	1.25
1	J	131	GLU	CD-OE2	9.70	1.36	1.25
1	O	131	GLU	CD-OE2	9.69	1.36	1.25

The worst 5 of 2531 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	210	ARG	NE-CZ-NH1	14.48	127.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	210	ARG	NE-CZ-NH1	14.45	127.53	120.30
1	G	210	ARG	NE-CZ-NH1	14.44	127.52	120.30
1	D	210	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	A	210	ARG	NE-CZ-NH1	14.41	127.50	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8219	0	7812	538	4
1	B	8219	0	7812	504	5
1	C	8219	0	7812	506	2
1	D	8219	0	7812	514	0
1	E	8219	0	7812	507	0
1	F	8219	0	7812	512	0
1	G	8219	0	7812	503	2
1	H	8219	0	7812	512	0
1	I	8219	0	7812	508	2
1	J	8219	0	7812	510	0
1	K	8219	0	7812	510	0
1	L	8219	0	7812	513	2
1	M	8219	0	7812	506	0
1	N	8219	0	7812	513	0
1	O	8219	0	7812	505	1
1	P	8219	0	7812	512	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

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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

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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	8056	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 31.

The worst 5 of 8056 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:O:427:THR:HA	1:O:436:MET:HE1	1.38	1.04
1:F:427:THR:HA	1:F:436:MET:HE1	1.41	1.03
1:C:427:THR:HA	1:C:436:MET:HE1	1.41	1.02
1:F:43:ARG:HG2	1:F:43:ARG:HH11	1.26	1.00
1:L:43:ARG:HG2	1:L:43:ARG:HH11	1.26	1.00

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	B	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	C	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	41	64
1	D	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	E	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	F	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	G	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	H	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	41	64
1	I	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	J	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	K	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	L	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	M	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	41	64
1	N	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
1	O	1018/1023 (100%)	952 (94%)	63 (6%)	3 (0%)	41	64
1	P	1018/1023 (100%)	953 (94%)	62 (6%)	3 (0%)	41	64
All	All	16288/16368 (100%)	15244 (94%)	996 (6%)	48 (0%)	41	64

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	B	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	C	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	D	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	E	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	F	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	G	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	H	872/872 (100%)	758 (87%)	114 (13%)	4	7
1	I	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	J	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	K	872/872 (100%)	758 (87%)	114 (13%)	4	7
1	L	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	M	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	N	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	O	872/872 (100%)	757 (87%)	115 (13%)	4	7
1	P	872/872 (100%)	758 (87%)	114 (13%)	4	7
All	All	13952/13952 (100%)	12115 (87%)	1837 (13%)	4	7

5 of 1837 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	49	GLN
1	P	377	LEU
1	J	986	ILE
1	P	211	ASP
1	N	903[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	739	HIS
1	P	739	HIS
1	N	128	ASN
1	O	363	HIS
1	F	394	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](#)

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	L	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	B	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	G	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	B	748	1	8,9,10	0.93	0	5,9,11	1.45	1 (20%)
1	CME	E	1021	1	8,9,10	1.08	0	5,9,11	1.46	0
1	CME	I	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	L	1021	1	8,9,10	1.07	0	5,9,11	1.47	0
1	CME	O	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	N	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	K	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	C	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	D	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	P	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	K	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	O	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	M	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	A	914	1	8,9,10	1.02	0	5,9,11	1.53	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	A	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	L	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	N	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	A	748	1	8,9,10	0.95	0	5,9,11	1.45	1 (20%)
1	CME	M	914	1	8,9,10	1.00	0	5,9,11	1.53	1 (20%)
1	CME	G	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	J	748	1	8,9,10	0.94	0	5,9,11	1.44	1 (20%)
1	CME	E	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	C	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	P	1021	1	8,9,10	1.08	0	5,9,11	1.46	0
1	CME	H	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	J	1021	1	8,9,10	1.07	0	5,9,11	1.47	0
1	CME	C	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	D	914	1	8,9,10	1.01	0	5,9,11	1.54	1 (20%)
1	CME	J	914	1	8,9,10	1.00	0	5,9,11	1.53	1 (20%)
1	CME	M	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	F	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	K	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	H	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	P	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	H	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	F	1021	1	8,9,10	1.08	0	5,9,11	1.46	0
1	CME	I	748	1	8,9,10	0.93	0	5,9,11	1.45	1 (20%)
1	CME	F	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	I	914	1	8,9,10	1.00	0	5,9,11	1.53	1 (20%)
1	CME	O	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	B	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	N	748	1	8,9,10	0.94	0	5,9,11	1.45	1 (20%)
1	CME	G	914	1	8,9,10	1.01	0	5,9,11	1.53	1 (20%)
1	CME	D	1021	1	8,9,10	1.07	0	5,9,11	1.46	0
1	CME	E	914	1	8,9,10	1.00	0	5,9,11	1.53	1 (20%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	H	1021	1	-	5/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	F	1021	1	-	5/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-
1	CME	F	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	3/5/8/10	-
1	CME	B	1021	1	-	5/5/8/10	-
1	CME	N	748	1	-	3/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	D	1021	1	-	5/5/8/10	-
1	CME	E	914	1	-	3/5/8/10	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	914	CME	CB-SG-SD	-2.71	96.80	103.82
1	K	914	CME	CB-SG-SD	-2.71	96.81	103.82
1	I	914	CME	CB-SG-SD	-2.70	96.81	103.82
1	H	914	CME	CB-SG-SD	-2.70	96.81	103.82
1	N	914	CME	CB-SG-SD	-2.70	96.81	103.82

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	A	1021	CME	SD-CE-CZ-OH

There are no ring outliers.

42 monomers are involved in 170 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	A	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	C	2001	1,4	11,11,12	1.26	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	D	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.56	2 (20%)
2	2FG	F	2001	1,4	11,11,12	1.28	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	N	2001	1,4	11,11,12	1.26	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	E	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	I	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	B	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	H	2001	1,4	11,11,12	1.26	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	G	2001	1,4	11,11,12	1.25	0	10,15,17	1.56	2 (20%)
2	2FG	J	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	M	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	K	2001	1,4	11,11,12	1.26	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	L	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	P	2001	1,4	11,11,12	1.27	1 (9%)	10,15,17	1.55	2 (20%)
2	2FG	O	2001	1,4	11,11,12	1.26	1 (9%)	10,15,17	1.55	2 (20%)

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	A	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
2	2FG	D	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	N	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	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	G	2001	1,4	1/1/4/5	2/2/19/22	0/1/1/1
2	2FG	J	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	K	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	P	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

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2001	2FG	C4-C5	2.04	1.57	1.53
2	N	2001	2FG	C4-C5	2.04	1.57	1.53
2	J	2001	2FG	C4-C5	2.03	1.57	1.53
2	M	2001	2FG	C4-C5	2.02	1.57	1.53
2	A	2001	2FG	C4-C5	2.02	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	2FG	O5-C5-C6	-3.76	101.32	107.20
2	N	2001	2FG	O5-C5-C6	-3.75	101.32	107.20
2	G	2001	2FG	O5-C5-C6	-3.75	101.32	107.20
2	B	2001	2FG	O5-C5-C6	-3.75	101.33	107.20
2	A	2001	2FG	O5-C5-C6	-3.74	101.33	107.20

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	2FG	C1

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Mol	Chain	Res	Type	Atom
2	B	2001	2FG	C1
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	A	2001	2FG	2	0
2	C	2001	2FG	2	0
2	D	2001	2FG	2	0
2	F	2001	2FG	2	0
2	N	2001	2FG	2	0
2	E	2001	2FG	2	0
2	I	2001	2FG	2	0
2	B	2001	2FG	2	0
2	H	2001	2FG	2	0
2	G	2001	2FG	2	0
2	J	2001	2FG	2	0
2	M	2001	2FG	2	0
2	K	2001	2FG	2	0
2	L	2001	2FG	2	0
2	P	2001	2FG	2	0
2	O	2001	2FG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1018/1023 (99%)	-0.42	9 (0%) 84 82	9, 32, 74, 100	3 (0%)
1	B	1018/1023 (99%)	-0.36	5 (0%) 91 89	7, 31, 72, 99	3 (0%)
1	C	1018/1023 (99%)	-0.39	0 100 100	6, 29, 70, 97	3 (0%)
1	D	1018/1023 (99%)	-0.28	9 (0%) 84 82	11, 35, 76, 100	3 (0%)
1	E	1018/1023 (99%)	-0.04	26 (2%) 56 50	23, 47, 84, 100	3 (0%)
1	F	1018/1023 (99%)	-0.41	4 (0%) 92 91	9, 33, 74, 100	3 (0%)
1	G	1018/1023 (99%)	-0.22	11 (1%) 80 78	13, 37, 77, 100	3 (0%)
1	H	1018/1023 (99%)	-0.10	22 (2%) 62 56	21, 45, 82, 100	3 (0%)
1	I	1018/1023 (99%)	-0.29	13 (1%) 77 73	17, 40, 80, 100	3 (0%)
1	J	1018/1023 (99%)	-0.42	3 (0%) 94 93	15, 38, 78, 100	3 (0%)
1	K	1018/1023 (99%)	-0.13	25 (2%) 57 51	25, 49, 85, 100	3 (0%)
1	L	1018/1023 (99%)	0.01	25 (2%) 57 51	24, 48, 85, 100	3 (0%)
1	M	1018/1023 (99%)	0.29	55 (5%) 25 20	27, 51, 86, 100	3 (0%)
1	N	1018/1023 (99%)	-0.33	7 (0%) 87 86	17, 40, 80, 100	3 (0%)
1	O	1018/1023 (99%)	-0.21	16 (1%) 72 68	17, 41, 80, 100	3 (0%)
1	P	1018/1023 (99%)	0.54	85 (8%) 11 8	32, 56, 90, 100	3 (0%)
All	All	16288/16368 (99%)	-0.17	315 (1%) 66 62	6, 42, 81, 100	48 (0%)

The worst 5 of 315 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	79	PRO	8.5
1	G	735	HIS	7.0
1	P	364	GLY	6.3
1	L	735	HIS	6.0
1	P	68	ALA	5.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	1021	10/11	0.82	0.26	53,74,100,100	0
1	CME	P	914	10/11	0.84	0.16	42,47,100,100	0
1	CME	H	1021	10/11	0.84	0.24	42,63,100,100	0
1	CME	L	748	10/11	0.86	0.17	43,63,100,100	0
1	CME	G	1021	10/11	0.88	0.19	34,55,100,100	0
1	CME	I	1021	10/11	0.89	0.18	38,59,100,100	0
1	CME	K	914	10/11	0.89	0.18	36,40,99,100	0
1	CME	K	1021	10/11	0.89	0.21	46,67,100,100	0
1	CME	C	748	10/11	0.90	0.19	23,44,86,96	0
1	CME	N	1021	10/11	0.90	0.20	38,59,100,100	0
1	CME	D	1021	10/11	0.91	0.16	32,54,100,100	0
1	CME	E	748	10/11	0.91	0.18	41,61,100,100	0
1	CME	E	1021	10/11	0.91	0.21	44,65,100,100	0
1	CME	F	1021	10/11	0.91	0.17	30,51,100,100	0
1	CME	M	1021	10/11	0.91	0.20	48,69,100,100	0
1	CME	G	748	10/11	0.91	0.19	31,51,93,100	0
1	CME	C	1021	10/11	0.91	0.16	26,48,96,96	0
1	CME	D	748	10/11	0.91	0.19	29,50,92,100	0
1	CME	M	914	10/11	0.92	0.14	38,42,100,100	0
1	CME	A	1021	10/11	0.92	0.20	30,51,100,100	0
1	CME	H	748	10/11	0.92	0.15	39,59,100,100	0
1	CME	O	748	10/11	0.92	0.26	36,56,98,100	0
1	CME	O	1021	10/11	0.92	0.18	39,60,100,100	0
1	CME	P	748	10/11	0.92	0.19	50,70,100,100	0
1	CME	K	748	10/11	0.92	0.21	43,64,100,100	0
1	CME	M	748	10/11	0.92	0.20	45,65,100,100	0
1	CME	L	1021	10/11	0.93	0.16	46,67,100,100	0
1	CME	O	914	10/11	0.93	0.15	28,33,92,100	0
1	CME	H	914	10/11	0.93	0.18	32,36,95,100	0
1	CME	B	748	10/11	0.93	0.12	25,46,87,98	0
1	CME	I	748	10/11	0.93	0.19	35,55,97,100	0
1	CME	B	1021	10/11	0.93	0.21	28,49,98,98	0
1	CME	I	914	10/11	0.94	0.15	27,32,91,100	0
1	CME	F	748	10/11	0.94	0.17	27,47,89,100	0
1	CME	J	748	10/11	0.94	0.15	33,53,95,100	0
1	CME	J	914	10/11	0.94	0.14	25,30,89,100	0
1	CME	N	914	10/11	0.94	0.12	27,32,91,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CME	L	914	10/11	0.94	0.12	35,40,99,100	0
1	CME	C	914	10/11	0.95	0.13	16,21,80,93	0
1	CME	N	748	10/11	0.95	0.15	35,55,97,100	0
1	CME	E	914	10/11	0.95	0.15	34,38,97,100	0
1	CME	G	914	10/11	0.95	0.13	24,28,87,100	0
1	CME	J	1021	10/11	0.95	0.20	36,57,100,100	0
1	CME	B	914	10/11	0.96	0.15	18,22,82,95	0
1	CME	A	748	10/11	0.96	0.12	27,47,89,100	0
1	CME	A	914	10/11	0.96	0.12	19,24,83,96	0
1	CME	D	914	10/11	0.96	0.14	22,27,86,99	0
1	CME	F	914	10/11	0.97	0.12	20,24,83,97	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, 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(\AA^2)	Q<0.9
4	NA	P	2004	1/1	0.37	0.24	67,67,67,67	0
4	NA	O	2004	1/1	0.63	0.14	53,53,53,53	0
4	NA	O	2005	1/1	0.64	0.17	37,37,37,37	0
4	NA	G	2005	1/1	0.69	0.17	32,32,32,32	0
4	NA	G	2004	1/1	0.69	0.15	48,48,48,48	0
4	NA	L	2004	1/1	0.71	0.16	60,60,60,60	0
4	NA	A	2004	1/1	0.74	0.16	44,44,44,44	0
4	NA	J	2004	1/1	0.74	0.28	50,50,50,50	0
4	NA	F	2004	1/1	0.76	0.21	44,44,44,44	0
4	NA	M	2004	1/1	0.80	0.36	62,62,62,62	0
4	NA	C	2004	1/1	0.80	0.13	41,41,41,41	0
4	NA	M	2005	1/1	0.83	0.31	46,46,46,46	0
3	MG	E	2003	1/1	0.84	0.10	39,39,39,39	0
4	NA	B	2004	1/1	0.85	0.15	42,42,42,42	0
4	NA	H	2004	1/1	0.85	0.10	56,56,56,56	0
2	2FG	P	2001	11/12	0.85	0.19	48,52,58,63	0
4	NA	I	2005	1/1	0.86	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	2003	1/1	0.86	0.13	27,27,27,27	0
4	NA	N	2004	1/1	0.87	0.10	52,52,52,52	0
3	MG	M	2002	1/1	0.87	0.11	43,43,43,43	0
3	MG	L	2003	1/1	0.88	0.12	40,40,40,40	0
2	2FG	L	2001	11/12	0.88	0.15	41,45,51,56	0
3	MG	N	2003	1/1	0.88	0.07	32,32,32,32	0
3	MG	O	2003	1/1	0.88	0.18	33,33,33,33	0
4	NA	K	2005	1/1	0.89	0.23	44,44,44,44	0
2	2FG	H	2001	11/12	0.89	0.14	37,41,48,52	0
2	2FG	M	2001	11/12	0.89	0.15	43,47,54,58	0
4	NA	D	2005	1/1	0.89	0.18	31,31,31,31	0
2	2FG	E	2001	11/12	0.90	0.14	39,43,49,54	0
4	NA	D	2004	1/1	0.90	0.14	47,47,47,47	0
3	MG	K	2003	1/1	0.90	0.14	41,41,41,41	0
4	NA	J	2005	1/1	0.90	0.18	34,34,34,34	0
2	2FG	F	2001	11/12	0.91	0.16	25,29,36,40	0
2	2FG	I	2001	11/12	0.91	0.13	33,37,43,48	0
4	NA	L	2005	1/1	0.91	0.25	44,44,44,44	0
4	NA	B	2005	1/1	0.92	0.22	26,26,26,26	0
4	NA	E	2004	1/1	0.92	0.26	58,58,58,58	0
2	2FG	A	2001	11/12	0.93	0.12	25,29,35,40	0
3	MG	M	2003	1/1	0.93	0.24	43,43,43,43	0
4	NA	K	2004	1/1	0.93	0.17	60,60,60,60	0
4	NA	N	2005	1/1	0.93	0.20	36,36,36,36	0
4	NA	E	2005	1/1	0.93	0.16	42,42,42,42	0
4	NA	I	2004	1/1	0.93	0.20	52,52,52,52	0
3	MG	J	2003	1/1	0.93	0.24	31,31,31,31	0
4	NA	C	2005	1/1	0.94	0.11	24,24,24,24	0
2	2FG	N	2001	11/12	0.94	0.12	33,37,43,48	0
3	MG	P	2002	1/1	0.94	0.17	47,47,47,47	0
2	2FG	J	2001	11/12	0.94	0.14	31,35,41,46	0
4	NA	A	2005	1/1	0.94	0.18	28,28,28,28	0
3	MG	H	2002	1/1	0.94	0.22	37,37,37,37	0
3	MG	I	2003	1/1	0.94	0.16	33,33,33,33	0
3	MG	C	2003	1/1	0.94	0.17	21,21,21,21	0
4	NA	P	2005	1/1	0.94	0.32	51,51,51,51	0
2	2FG	O	2001	11/12	0.95	0.14	34,38,44,49	0
2	2FG	B	2001	11/12	0.95	0.20	23,27,34,38	0
2	2FG	G	2001	11/12	0.95	0.16	29,33,40,44	0
4	NA	H	2005	1/1	0.95	0.24	40,40,40,40	0
3	MG	I	2002	1/1	0.95	0.16	32,32,32,32	0
3	MG	F	2003	1/1	0.96	0.10	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	G	2003	1/1	0.96	0.08	29,29,29,29	0
2	2FG	D	2001	11/12	0.96	0.14	28,32,38,43	0
3	MG	H	2003	1/1	0.96	0.07	37,37,37,37	0
2	2FG	K	2001	11/12	0.96	0.13	41,45,52,56	0
4	NA	F	2005	1/1	0.97	0.14	28,28,28,28	0
3	MG	G	2002	1/1	0.97	0.24	29,29,29,29	0
3	MG	B	2003	1/1	0.97	0.10	23,23,23,23	0
2	2FG	C	2001	11/12	0.97	0.12	22,26,32,37	0
3	MG	K	2002	1/1	0.97	0.17	41,41,41,41	0
3	MG	O	2002	1/1	0.97	0.26	33,33,33,33	0
3	MG	D	2002	1/1	0.97	0.13	27,27,27,27	0
3	MG	A	2003	1/1	0.98	0.14	24,24,24,24	0
3	MG	F	2002	1/1	0.98	0.19	25,25,25,25	0
3	MG	L	2002	1/1	0.98	0.17	40,40,40,40	0
3	MG	P	2003	1/1	0.98	0.12	48,48,48,48	0
3	MG	B	2002	1/1	0.98	0.31	23,23,23,23	0
3	MG	A	2002	1/1	0.98	0.10	24,24,24,24	0
3	MG	J	2002	1/1	0.98	0.10	30,30,30,30	0
3	MG	N	2002	1/1	0.98	0.16	32,32,32,32	0
3	MG	E	2002	1/1	0.98	0.18	38,38,38,38	0
3	MG	C	2002	1/1	0.99	0.23	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.