



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 11:48 PM EDT

PDB ID : 1PX3  
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (G794A)  
Authors : Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.  
Deposited on : 2003-07-02  
Resolution : 1.60 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](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 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 : 2.23.2  
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) : 2.23.2

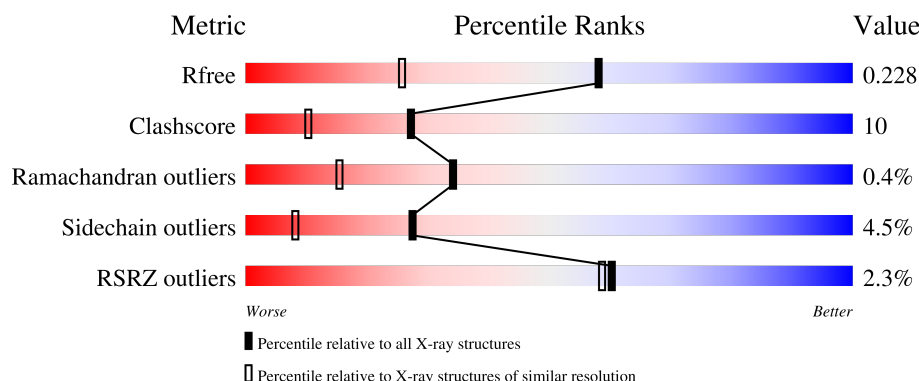
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	
1	B	1023	
1	C	1023	
1	D	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
4	DMS	A	8404	-	-	X	-
4	DMS	C	8425	-	-	X	-
4	DMS	D	8703	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36619 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	1010	Total	C	N	O	S	0	0	0
			8119	5135	1439	1507	38			
1	B	1009	Total	C	N	O	S	0	0	0
			8114	5132	1438	1506	38			
1	C	1007	Total	C	N	O	S	0	0	0
			8095	5120	1433	1504	38			
1	D	1008	Total	C	N	O	S	0	0	0
			8103	5126	1434	1505	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P00722
A	2	SER	-	cloning artifact	UNP P00722
A	3	HIS	-	cloning artifact	UNP P00722
A	4	MET	-	cloning artifact	UNP P00722
A	5	LEU	-	cloning artifact	UNP P00722
A	6	GLU	-	cloning artifact	UNP P00722
A	7	ASP	-	cloning artifact	UNP P00722
A	8	PRO	-	cloning artifact	UNP P00722
A	794	ALA	GLY	engineered mutation	UNP P00722
B	1	GLY	-	cloning artifact	UNP P00722
B	2	SER	-	cloning artifact	UNP P00722
B	3	HIS	-	cloning artifact	UNP P00722
B	4	MET	-	cloning artifact	UNP P00722
B	5	LEU	-	cloning artifact	UNP P00722
B	6	GLU	-	cloning artifact	UNP P00722
B	7	ASP	-	cloning artifact	UNP P00722
B	8	PRO	-	cloning artifact	UNP P00722
B	794	ALA	GLY	engineered mutation	UNP P00722
C	1	GLY	-	cloning artifact	UNP P00722
C	2	SER	-	cloning artifact	UNP P00722
C	3	HIS	-	cloning artifact	UNP P00722

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	cloning artifact	UNP P00722
C	5	LEU	-	cloning artifact	UNP P00722
C	6	GLU	-	cloning artifact	UNP P00722
C	7	ASP	-	cloning artifact	UNP P00722
C	8	PRO	-	cloning artifact	UNP P00722
C	794	ALA	GLY	engineered mutation	UNP P00722
D	1	GLY	-	cloning artifact	UNP P00722
D	2	SER	-	cloning artifact	UNP P00722
D	3	HIS	-	cloning artifact	UNP P00722
D	4	MET	-	cloning artifact	UNP P00722
D	5	LEU	-	cloning artifact	UNP P00722
D	6	GLU	-	cloning artifact	UNP P00722
D	7	ASP	-	cloning artifact	UNP P00722
D	8	PRO	-	cloning artifact	UNP P00722
D	794	ALA	GLY	engineered mutation	UNP P00722

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	2	Total Mg 2 2	0	0
2	C	4	Total Mg 4 4	0	0
2	D	3	Total Mg 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0

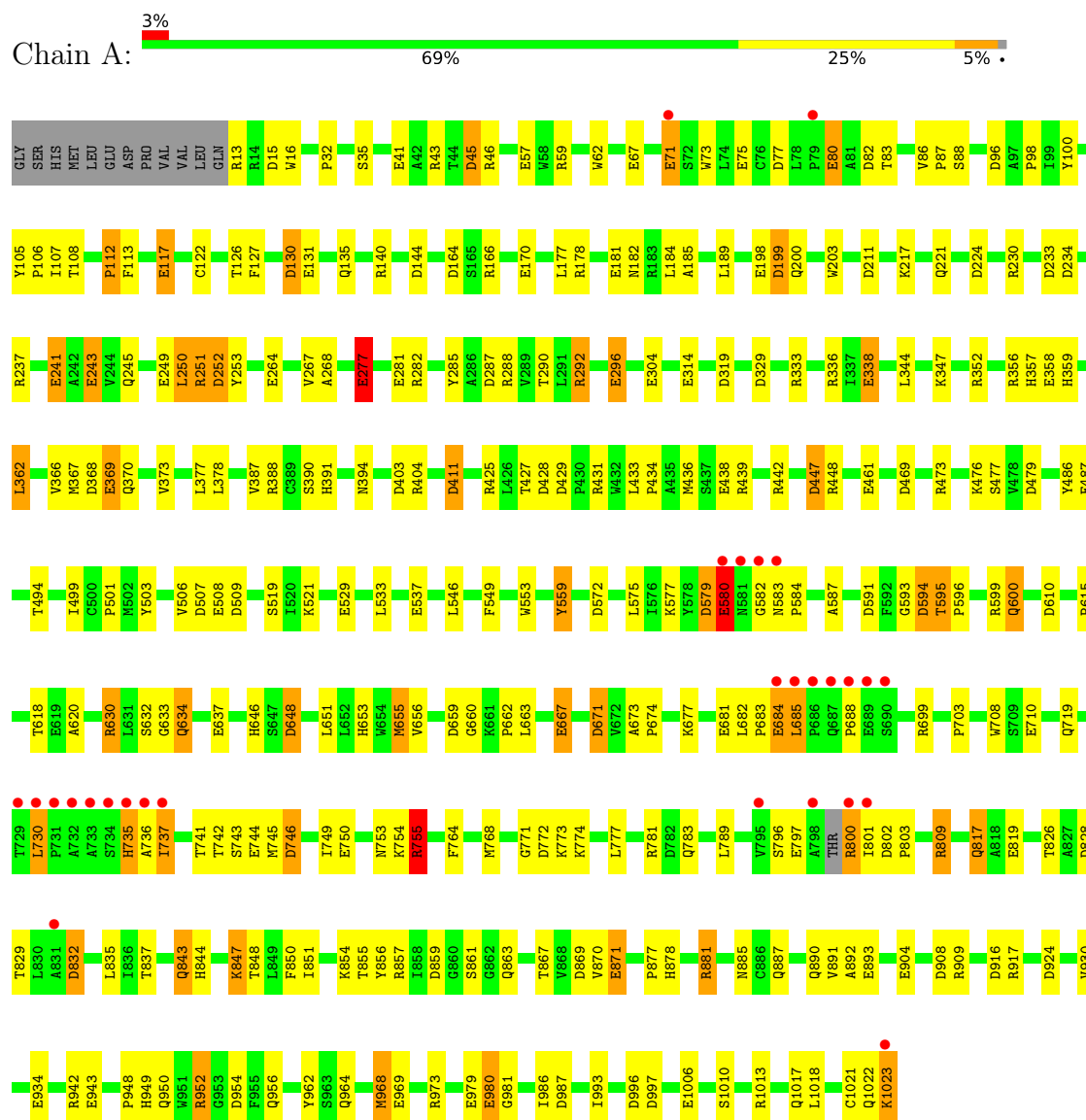
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	916	Total O 916 916	0	0
5	B	985	Total O 985 985	0	0
5	C	935	Total O 935 935	0	0
5	D	984	Total O 984 984	0	0

### 3 Residue-property plots

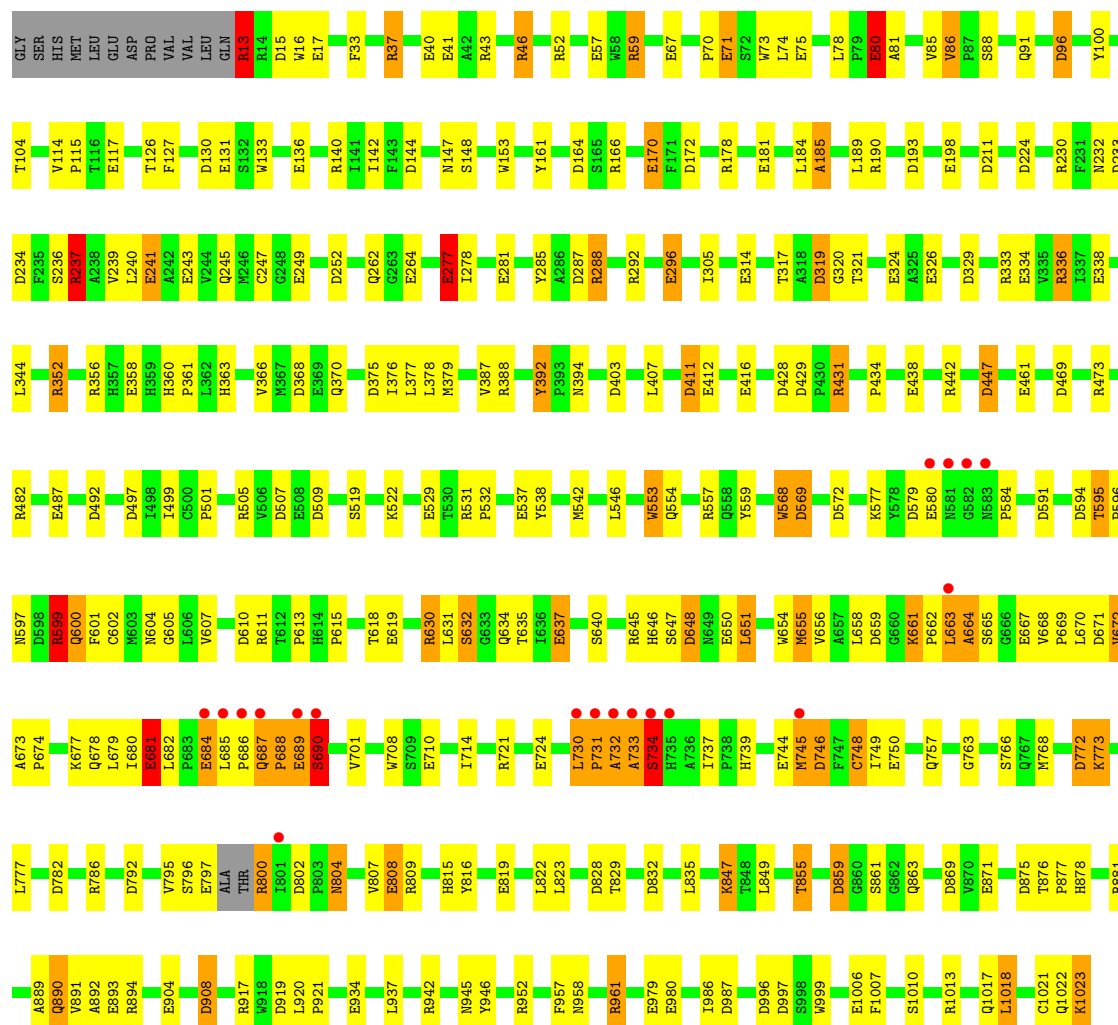
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: beta-galactosidase

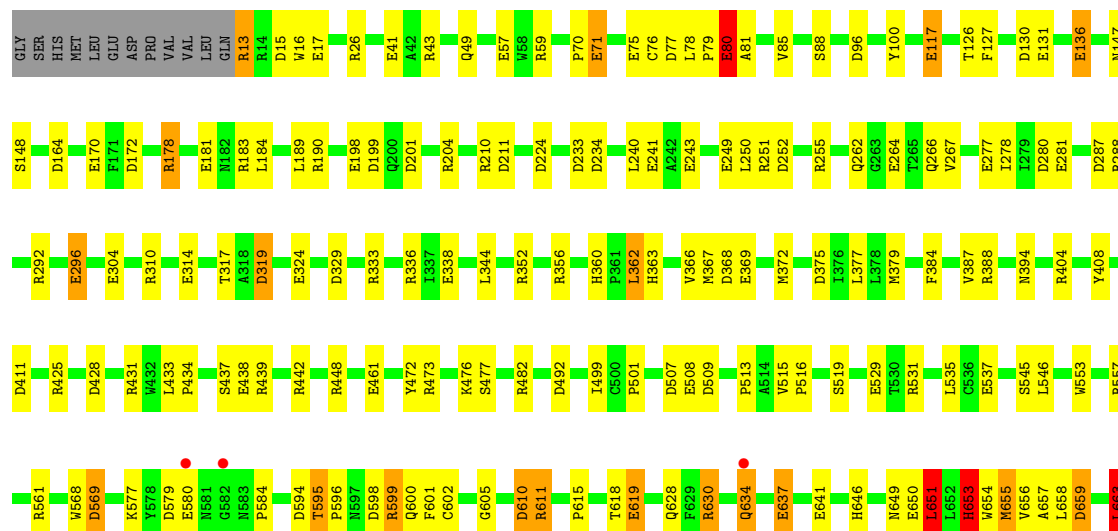


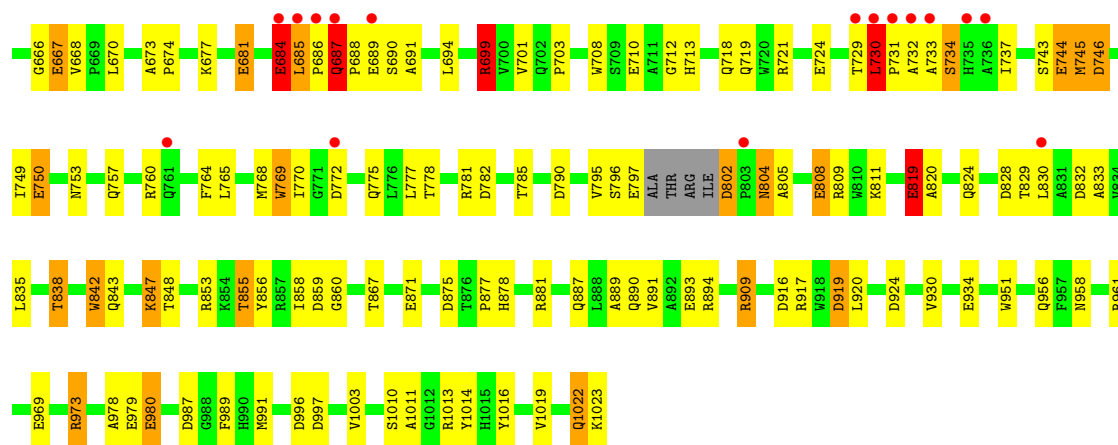
- Molecule 1: beta-galactosidase



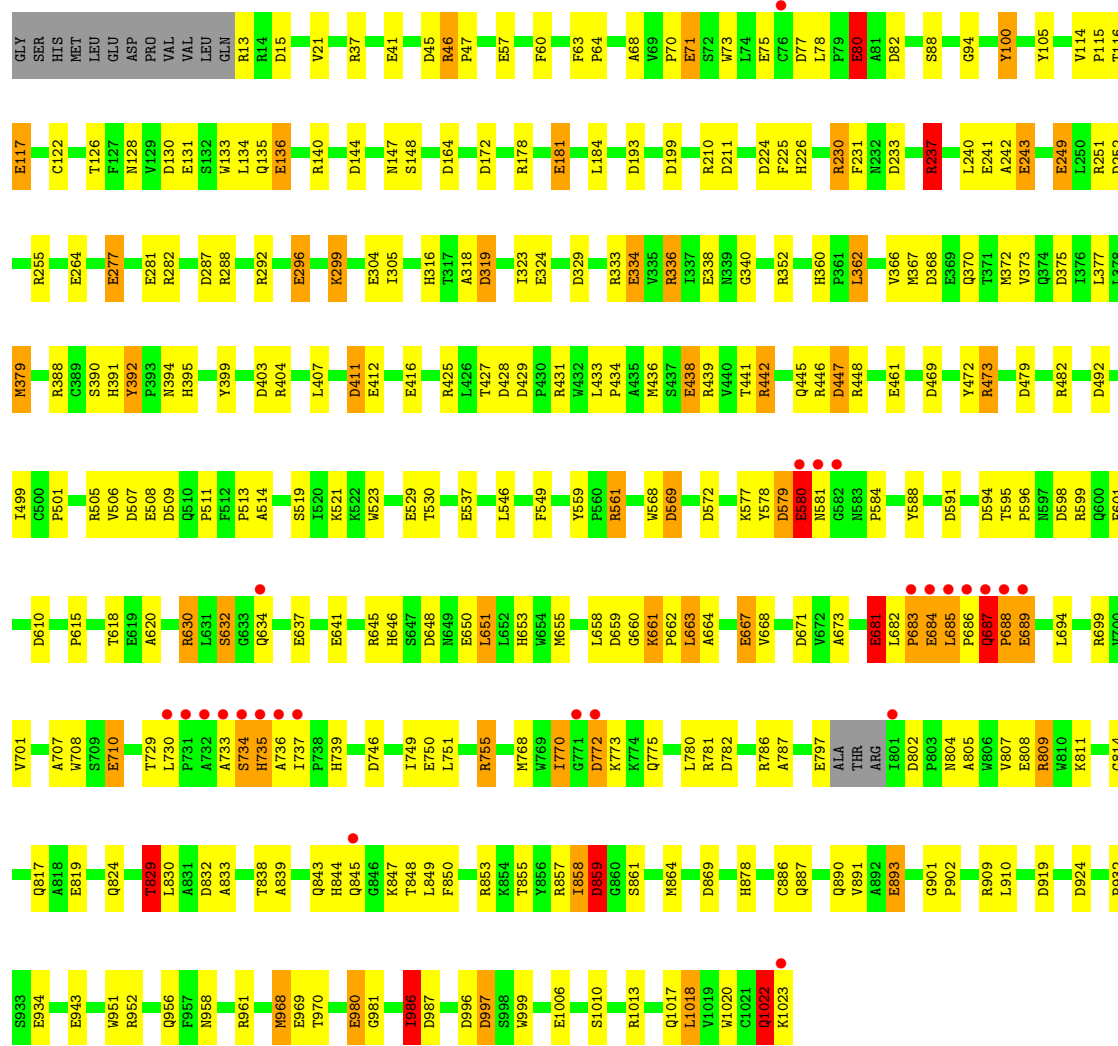


● Molecule 1: beta-galactosidase





• Molecule 1: beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.70Å 168.59Å 200.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 1.60 21.69 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.70-1.60) 88.2 (21.69-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.192 , 0.243 0.180 , 0.228	Depositor DCC
$R_{free}$ test set	8858 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 83.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8122e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, DMS, 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	1.12	44/8360 (0.5%)	1.67	159/11404 (1.4%)
1	B	1.15	55/8355 (0.7%)	1.64	152/11397 (1.3%)
1	C	1.13	50/8336 (0.6%)	1.66	162/11372 (1.4%)
1	D	1.13	45/8344 (0.5%)	1.68	172/11383 (1.5%)
All	All	1.13	194/33395 (0.6%)	1.66	645/45556 (1.4%)

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	C	1	0

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	9.86	1.36	1.25
1	A	249	GLU	CD-OE2	9.72	1.36	1.25
1	D	136	GLU	CD-OE2	8.94	1.35	1.25
1	D	893	GLU	CD-OE2	8.89	1.35	1.25
1	C	650	GLU	CD-OE2	8.83	1.35	1.25

The worst 5 of 645 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	ARG	NE-CZ-NH1	24.71	132.65	120.30
1	C	699	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	C	599	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	D	630	ARG	NE-CZ-NH1	16.23	128.41	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	ARG	NE-CZ-NH1	16.07	128.33	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	733	ALA	CA

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	8119	0	7710	160	0
1	B	8114	0	7705	173	0
1	C	8095	0	7681	156	0
1	D	8103	0	7692	154	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	88	0	132	19	0
4	B	72	0	108	7	0
4	C	84	0	126	17	0
4	D	96	0	144	15	0
5	A	916	0	0	20	0
5	B	985	0	0	15	0
5	C	935	0	0	14	0
5	D	984	0	0	17	0
All	All	36619	0	31298	645	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 10.



The worst 5 of 645 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)
4:B:8601:DMS:C2	4:B:8601:DMS:S	2.03	1.47
1:B:376:ILE:HA	1:B:379:MET:HE2	1.26	1.12
1:C:649:ASN:HA	4:C:8425:DMS:H12	1.37	1.06
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.84	0.92
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.01	0.91

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	1006/1023 (98%)	972 (97%)	33 (3%)	1 (0%)	51 29
1	B	1005/1023 (98%)	962 (96%)	36 (4%)	7 (1%)	22 7
1	C	1003/1023 (98%)	968 (96%)	32 (3%)	3 (0%)	41 21
1	D	1004/1023 (98%)	961 (96%)	39 (4%)	4 (0%)	34 15
All	All	4018/4092 (98%)	3863 (96%)	140 (4%)	15 (0%)	34 15

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	B	732	ALA
1	B	734	SER
1	D	688	PRO

### 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	863/875 (99%)	831 (96%)	32 (4%)	34	11
1	B	863/875 (99%)	821 (95%)	42 (5%)	25	6
1	C	861/875 (98%)	824 (96%)	37 (4%)	29	9
1	D	862/875 (98%)	819 (95%)	43 (5%)	24	6
All	All	3449/3500 (98%)	3295 (96%)	154 (4%)	27	8

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	249	GLU
1	D	772	ASP
1	D	362	LEU
1	D	655	MET
1	D	956	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	878	HIS
1	D	628	GLN
1	C	977	HIS
1	D	135	GLN
1	D	704	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 28 are monoatomic - leaving 85 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
4	DMS	A	8502	-	3,3,3	2.09	1 (33%)	3,3,3	1.00	0
4	DMS	D	8404	-	3,3,3	1.18	0	3,3,3	0.51	0
4	DMS	B	8504	-	3,3,3	0.37	0	3,3,3	0.11	0
4	DMS	A	8602	-	3,3,3	0.72	0	3,3,3	0.22	0
4	DMS	C	8601	-	3,3,3	0.65	0	3,3,3	0.52	0
4	DMS	C	8504	-	3,3,3	1.23	0	3,3,3	1.08	0
4	DMS	D	8421	-	3,3,3	0.32	0	3,3,3	0.49	0
4	DMS	B	8601	-	3,3,3	2.49	1 (33%)	3,3,3	0.79	0
4	DMS	D	8402	-	3,3,3	1.36	0	3,3,3	0.23	0
4	DMS	D	8401	-	3,3,3	1.66	1 (33%)	3,3,3	0.12	0
4	DMS	A	8414	-	3,3,3	0.40	0	3,3,3	0.20	0
4	DMS	A	8504	-	3,3,3	0.93	0	3,3,3	0.41	0
4	DMS	C	8417	-	3,3,3	0.27	0	3,3,3	0.42	0
4	DMS	C	8501	-	3,3,3	1.53	1 (33%)	3,3,3	0.77	0
4	DMS	C	8421	-	3,3,3	1.22	0	3,3,3	0.57	0
4	DMS	A	8404	-	3,3,3	1.48	1 (33%)	3,3,3	0.58	0
4	DMS	C	8409	-	3,3,3	2.15	1 (33%)	3,3,3	0.32	0
4	DMS	A	8501	-	3,3,3	0.76	0	3,3,3	0.44	0
4	DMS	C	8602	-	3,3,3	0.56	0	3,3,3	0.22	0
4	DMS	D	8414	-	3,3,3	0.40	0	3,3,3	0.55	0
4	DMS	D	8703	-	3,3,3	0.82	0	3,3,3	0.27	0
4	DMS	C	8425	3	3,3,3	1.05	0	3,3,3	0.12	0
4	DMS	A	8421	-	3,3,3	0.98	0	3,3,3	0.77	0
4	DMS	A	8403	-	3,3,3	1.77	1 (33%)	3,3,3	0.65	0
4	DMS	A	8409	-	3,3,3	2.35	2 (66%)	3,3,3	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	8401	-	3,3,3	1.21	0	3,3,3	0.52	0
4	DMS	A	8402	-	3,3,3	1.20	0	3,3,3	0.75	0
4	DMS	B	8502	-	3,3,3	1.49	0	3,3,3	1.22	1 (33%)
4	DMS	D	8701	-	3,3,3	1.51	1 (33%)	3,3,3	0.46	0
4	DMS	D	8410	-	3,3,3	1.93	1 (33%)	3,3,3	0.24	0
4	DMS	A	8411	-	3,3,3	1.50	0	3,3,3	0.49	0
4	DMS	B	8402	-	3,3,3	1.80	1 (33%)	3,3,3	1.27	1 (33%)
4	DMS	D	8413	-	3,3,3	0.81	0	3,3,3	0.03	0
4	DMS	A	8425	3	3,3,3	1.22	0	3,3,3	0.70	0
4	DMS	B	8416	-	3,3,3	1.00	0	3,3,3	0.24	0
4	DMS	B	8404	-	3,3,3	0.99	0	3,3,3	0.51	0
4	DMS	C	8403	-	3,3,3	1.42	1 (33%)	3,3,3	0.33	0
4	DMS	A	8408	-	3,3,3	0.55	0	3,3,3	0.34	0
4	DMS	D	8705	-	3,3,3	1.94	1 (33%)	3,3,3	0.30	0
4	DMS	D	8508	-	3,3,3	1.39	0	3,3,3	0.90	0
4	DMS	B	8508	-	3,3,3	2.06	1 (33%)	3,3,3	0.81	0
4	DMS	B	8411	-	3,3,3	0.54	0	3,3,3	0.82	0
4	DMS	B	8412	-	3,3,3	0.88	0	3,3,3	0.25	0
4	DMS	D	8403	-	3,3,3	1.28	0	3,3,3	0.35	0
4	DMS	C	8404	-	3,3,3	1.29	0	3,3,3	1.11	0
4	DMS	A	8405	-	3,3,3	1.29	1 (33%)	3,3,3	0.44	0
4	DMS	D	8408	-	3,3,3	1.31	1 (33%)	3,3,3	0.26	0
4	DMS	C	8405	-	3,3,3	2.61	2 (66%)	3,3,3	0.27	0
4	DMS	B	8417	-	3,3,3	0.82	0	3,3,3	0.52	0
4	DMS	C	8414	-	3,3,3	1.75	1 (33%)	3,3,3	1.19	0
4	DMS	B	8421	-	3,3,3	0.58	0	3,3,3	0.38	0
4	DMS	A	8503	-	3,3,3	1.06	0	3,3,3	0.74	0
4	DMS	D	8501	-	3,3,3	0.84	0	3,3,3	0.37	0
4	DMS	B	8401	-	3,3,3	0.96	0	3,3,3	0.43	0
4	DMS	C	8401	-	3,3,3	1.74	1 (33%)	3,3,3	0.38	0
4	DMS	B	8409	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
4	DMS	D	8409	-	3,3,3	1.96	1 (33%)	3,3,3	1.39	1 (33%)
4	DMS	D	8416	-	3,3,3	0.26	0	3,3,3	0.54	0
4	DMS	C	8408	-	3,3,3	0.75	0	3,3,3	1.10	0
4	DMS	A	8417	-	3,3,3	1.00	0	3,3,3	0.79	0
4	DMS	B	8405	-	3,3,3	2.22	1 (33%)	3,3,3	0.28	0
4	DMS	C	8410	-	3,3,3	0.69	0	3,3,3	0.16	0
4	DMS	D	8417	-	3,3,3	0.46	0	3,3,3	0.21	0
4	DMS	B	8414	-	3,3,3	1.01	0	3,3,3	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	D	8406	-	3,3,3	0.86	0	3,3,3	0.53	0
4	DMS	A	8416	-	3,3,3	2.03	2 (66%)	3,3,3	0.62	0
4	DMS	D	8412	-	3,3,3	1.63	1 (33%)	3,3,3	0.54	0
4	DMS	B	8408	-	3,3,3	1.26	0	3,3,3	0.08	0
4	DMS	D	8425	3	3,3,3	0.93	0	3,3,3	0.37	0
4	DMS	D	8411	-	3,3,3	1.36	0	3,3,3	0.22	0
4	DMS	C	8503	-	3,3,3	0.85	0	3,3,3	1.43	1 (33%)
4	DMS	B	8425	3	3,3,3	1.12	0	3,3,3	0.40	0
4	DMS	A	8406	-	3,3,3	1.78	1 (33%)	3,3,3	0.42	0
4	DMS	C	8413	-	3,3,3	0.71	0	3,3,3	0.29	0
4	DMS	A	8419	-	3,3,3	1.10	0	3,3,3	0.40	0
4	DMS	B	8403	-	3,3,3	1.10	0	3,3,3	0.13	0
4	DMS	A	8412	-	3,3,3	2.09	1 (33%)	3,3,3	0.47	0
4	DMS	C	8412	-	3,3,3	1.20	0	3,3,3	1.37	1 (33%)
4	DMS	C	8416	-	3,3,3	0.67	0	3,3,3	0.31	0
4	DMS	A	8410	-	3,3,3	0.58	0	3,3,3	0.55	0
4	DMS	C	8402	-	3,3,3	2.22	1 (33%)	3,3,3	0.17	0
4	DMS	D	8419	-	3,3,3	0.59	0	3,3,3	0.49	0
4	DMS	D	8405	-	3,3,3	0.79	0	3,3,3	0.49	0
4	DMS	C	8411	-	3,3,3	1.13	0	3,3,3	0.30	0
4	DMS	D	8503	-	3,3,3	0.68	0	3,3,3	0.79	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8409	DMS	O-S	4.60	1.81	1.50
4	C	8405	DMS	O-S	3.93	1.76	1.50
4	B	8601	DMS	C2-S	3.77	2.03	1.75
4	C	8409	DMS	O-S	3.66	1.75	1.50
4	B	8405	DMS	O-S	3.53	1.74	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8503	DMS	C2-S-C1	2.39	110.74	98.44
4	D	8409	DMS	C2-S-C1	2.36	110.58	98.44
4	C	8412	DMS	C2-S-C1	2.34	110.50	98.44
4	B	8402	DMS	C2-S-C1	2.16	109.55	98.44
4	B	8502	DMS	C2-S-C1	2.11	109.32	98.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8502	DMS	3	0
4	B	8504	DMS	2	0
4	A	8602	DMS	1	0
4	C	8601	DMS	2	0
4	D	8421	DMS	2	0
4	B	8601	DMS	1	0
4	A	8404	DMS	5	0
4	C	8602	DMS	1	0
4	D	8703	DMS	5	0
4	C	8425	DMS	7	0
4	A	8403	DMS	1	0
4	A	8425	DMS	2	0
4	D	8705	DMS	1	0
4	B	8411	DMS	1	0
4	B	8412	DMS	1	0
4	D	8403	DMS	1	0
4	A	8503	DMS	1	0
4	B	8409	DMS	1	0
4	C	8410	DMS	1	0
4	D	8417	DMS	1	0
4	D	8406	DMS	1	0
4	A	8416	DMS	2	0
4	D	8412	DMS	2	0
4	C	8503	DMS	2	0
4	C	8413	DMS	1	0
4	B	8403	DMS	1	0
4	A	8412	DMS	1	0
4	C	8412	DMS	1	0
4	A	8410	DMS	3	0
4	C	8402	DMS	1	0
4	D	8419	DMS	1	0
4	C	8411	DMS	1	0
4	D	8503	DMS	1	0

## 5.7 Other polymers ⓘ

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, 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	1010/1023 (98%)	-0.37	28 (2%) 53 50	9, 18, 47, 97	0
1	B	1009/1023 (98%)	-0.40	19 (1%) 66 65	9, 17, 44, 94	0
1	C	1007/1023 (98%)	-0.40	19 (1%) 66 65	8, 17, 45, 99	0
1	D	1008/1023 (98%)	-0.40	25 (2%) 57 55	9, 17, 46, 94	0
All	All	4034/4092 (98%)	-0.39	91 (2%) 60 59	8, 17, 45, 99	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	ALA	7.5
1	B	733	ALA	7.4
1	A	730	LEU	7.3
1	C	732	ALA	7.2
1	B	731	PRO	6.9

### 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 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	A	3005	1/1	0.74	0.12	42,42,42,42	0
2	MG	C	3004	1/1	0.78	0.10	52,52,52,52	0
4	DMS	C	8504	4/4	0.82	0.14	36,68,72,73	0
4	DMS	C	8503	4/4	0.84	0.16	30,35,46,59	0
4	DMS	B	8425	4/4	0.86	0.12	32,33,41,56	0
4	DMS	C	8413	4/4	0.86	0.21	42,69,100,100	0
4	DMS	A	8421	4/4	0.87	0.26	35,58,84,100	0
4	DMS	D	8419	4/4	0.87	0.20	54,72,74,95	0
4	DMS	D	8413	4/4	0.88	0.17	28,56,73,100	0
4	DMS	D	8416	4/4	0.89	0.16	25,43,52,77	0
4	DMS	D	8417	4/4	0.90	0.13	26,32,41,100	0
4	DMS	C	8602	4/4	0.90	0.14	25,45,68,100	0
4	DMS	D	8425	4/4	0.90	0.15	16,27,33,36	4
4	DMS	D	8503	4/4	0.90	0.19	43,44,59,100	0
4	DMS	D	8703	4/4	0.90	0.18	37,58,59,100	0
4	DMS	D	8705	4/4	0.90	0.17	18,50,52,67	0
3	NA	D	3104	1/1	0.91	0.09	35,35,35,35	0
4	DMS	A	8419	4/4	0.91	0.20	65,67,69,100	0
4	DMS	B	8508	4/4	0.91	0.12	36,41,50,64	0
4	DMS	B	8417	4/4	0.92	0.15	31,39,48,62	0
4	DMS	D	8501	4/4	0.92	0.08	25,33,43,59	0
4	DMS	D	8409	4/4	0.92	0.11	24,33,33,40	0
4	DMS	A	8503	4/4	0.92	0.20	41,50,94,100	0
4	DMS	D	8421	4/4	0.92	0.19	42,61,71,100	0
4	DMS	C	8417	4/4	0.93	0.10	33,36,45,63	0
4	DMS	A	8502	4/4	0.93	0.17	23,38,48,83	0
4	DMS	D	8508	4/4	0.93	0.10	39,47,52,59	0
4	DMS	A	8425	4/4	0.93	0.14	29,37,46,51	0
4	DMS	C	8601	4/4	0.93	0.15	49,50,73,100	0
4	DMS	A	8404	4/4	0.94	0.10	19,26,41,49	0
4	DMS	B	8404	4/4	0.94	0.11	24,29,41,100	0
4	DMS	B	8409	4/4	0.94	0.09	21,26,39,44	0
4	DMS	A	8417	4/4	0.94	0.12	26,26,68,100	0
4	DMS	B	8421	4/4	0.95	0.11	32,60,64,68	0
3	NA	D	3103	1/1	0.95	0.09	36,36,36,36	0
4	DMS	A	8406	4/4	0.95	0.12	12,45,59,77	0
4	DMS	B	8601	4/4	0.95	0.14	33,36,39,39	0
4	DMS	A	8416	4/4	0.95	0.19	20,39,63,71	0
4	DMS	C	8414	4/4	0.95	0.11	23,25,34,42	0
3	NA	A	3103	1/1	0.95	0.10	38,38,38,38	0
4	DMS	C	8501	4/4	0.95	0.10	27,31,39,56	0
4	DMS	B	8502	4/4	0.96	0.10	22,27,37,41	0
4	DMS	B	8504	4/4	0.96	0.10	30,33,44,82	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	D	8406	4/4	0.96	0.09	21,25,26,42	0
4	DMS	A	8414	4/4	0.96	0.13	22,43,69,100	0
4	DMS	D	8410	4/4	0.96	0.10	40,52,57,60	0
3	NA	B	3104	1/1	0.96	0.11	33,33,33,33	0
4	DMS	D	8414	4/4	0.96	0.15	33,50,100,100	0
4	DMS	C	8409	4/4	0.96	0.08	29,30,33,36	0
3	NA	C	3104	1/1	0.96	0.08	28,28,28,28	0
2	MG	D	3005	1/1	0.96	0.09	26,26,26,26	0
4	DMS	C	8416	4/4	0.96	0.26	44,51,52,100	0
4	DMS	B	8416	4/4	0.96	0.12	32,33,42,49	0
4	DMS	C	8421	4/4	0.96	0.16	41,44,60,65	0
4	DMS	C	8425	4/4	0.96	0.21	44,50,66,88	0
4	DMS	A	8409	4/4	0.96	0.09	23,25,28,41	0
4	DMS	A	8412	4/4	0.96	0.14	28,33,41,100	0
4	DMS	A	8501	4/4	0.96	0.08	20,25,41,42	0
3	NA	A	3104	1/1	0.97	0.09	29,29,29,29	0
4	DMS	A	8410	4/4	0.97	0.11	41,49,78,100	0
4	DMS	D	8404	4/4	0.97	0.09	22,27,43,76	0
4	DMS	A	8411	4/4	0.97	0.10	25,34,36,44	0
4	DMS	C	8404	4/4	0.97	0.07	17,23,30,37	0
4	DMS	C	8405	4/4	0.97	0.11	28,31,31,36	0
4	DMS	C	8408	4/4	0.97	0.09	26,28,34,40	0
3	NA	D	3101	1/1	0.97	0.07	24,24,24,24	0
4	DMS	A	8408	4/4	0.97	0.10	21,34,39,80	0
4	DMS	C	8411	4/4	0.98	0.11	25,31,31,100	0
4	DMS	C	8412	4/4	0.98	0.10	30,37,38,41	0
4	DMS	A	8504	4/4	0.98	0.07	23,40,44,77	0
4	DMS	D	8411	4/4	0.98	0.12	31,33,34,100	0
4	DMS	A	8602	4/4	0.98	0.15	35,49,98,100	0
4	DMS	B	8401	4/4	0.98	0.09	16,19,21,23	0
4	DMS	B	8402	4/4	0.98	0.07	16,16,21,22	0
2	MG	C	3006	1/1	0.98	0.08	31,31,31,31	0
4	DMS	B	8405	4/4	0.98	0.11	31,36,37,40	0
4	DMS	B	8408	4/4	0.98	0.11	33,34,35,100	0
4	DMS	A	8403	4/4	0.98	0.06	21,23,28,29	0
4	DMS	B	8412	4/4	0.98	0.06	26,29,33,36	0
4	DMS	B	8414	4/4	0.98	0.13	25,36,42,46	0
3	NA	B	3101	1/1	0.98	0.07	17,17,17,17	0
4	DMS	D	8701	4/4	0.98	0.09	15,18,24,53	0
4	DMS	D	8403	4/4	0.98	0.07	21,26,28,31	0
4	DMS	C	8410	4/4	0.98	0.11	26,40,42,49	0
4	DMS	C	8401	4/4	0.99	0.05	14,15,19,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	D	8401	4/4	0.99	0.07	14,17,19,20	0
4	DMS	D	8402	4/4	0.99	0.05	12,20,21,23	0
4	DMS	C	8402	4/4	0.99	0.05	16,16,23,25	0
4	DMS	C	8403	4/4	0.99	0.12	16,21,24,30	0
4	DMS	D	8405	4/4	0.99	0.06	24,25,39,45	0
3	NA	C	3102	1/1	0.99	0.06	14,14,14,14	0
4	DMS	D	8408	4/4	0.99	0.06	18,30,35,45	0
4	DMS	B	8403	4/4	0.99	0.09	22,23,28,30	0
3	NA	C	3103	1/1	0.99	0.09	27,27,27,27	0
2	MG	B	3002	1/1	0.99	0.04	15,15,15,15	0
4	DMS	D	8412	4/4	0.99	0.06	27,27,35,100	0
3	NA	A	3101	1/1	0.99	0.07	23,23,23,23	0
3	NA	D	3102	1/1	0.99	0.04	12,12,12,12	0
4	DMS	B	8411	4/4	0.99	0.10	33,34,34,46	0
3	NA	A	3102	1/1	0.99	0.04	12,12,12,12	0
2	MG	A	3002	1/1	0.99	0.04	17,17,17,17	0
4	DMS	A	8401	4/4	0.99	0.10	12,15,15,17	0
4	DMS	A	8402	4/4	0.99	0.05	15,17,23,36	0
2	MG	A	3001	1/1	0.99	0.04	17,17,17,17	0
2	MG	D	3001	1/1	0.99	0.03	14,14,14,14	0
4	DMS	A	8405	4/4	0.99	0.06	25,25,26,29	0
3	NA	B	3103	1/1	0.99	0.06	26,26,26,26	0
2	MG	D	3002	1/1	0.99	0.03	16,16,16,16	0
3	NA	C	3101	1/1	0.99	0.06	18,18,18,18	0
3	NA	B	3102	1/1	1.00	0.06	13,13,13,13	0
2	MG	C	3001	1/1	1.00	0.10	15,15,15,15	0
2	MG	C	3002	1/1	1.00	0.03	13,13,13,13	0
2	MG	B	3001	1/1	1.00	0.09	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.