



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 09:00 PM EDT

PDB ID : 3I3E  
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (M542A)  
Authors : Dugdale, M.L.; Dymianiw, D.; Minhas, B.; Huber, R.E.  
Deposited on : 2009-06-30  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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

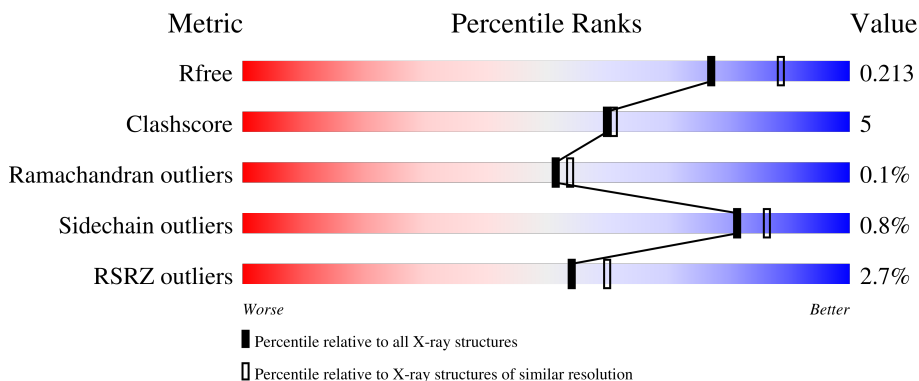
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	 3% 86% 13% .
1	B	1023	 2% 87% 11% .
1	C	1023	 3% 87% 11% .
1	D	1023	 3% 88% 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
4	DMS	D	8413	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 36653 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	1011	8122	5136	1440	1509	37	0	0	0
1	B	1010	8113	5130	1438	1508	37	0	0	0
1	C	1011	8122	5136	1440	1509	37	0	0	0
1	D	1011	8122	5136	1440	1509	37	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B8LFD6
A	2	SER	-	expression tag	UNP B8LFD6
A	3	HIS	-	expression tag	UNP B8LFD6
A	4	MET	-	expression tag	UNP B8LFD6
A	5	LEU	-	expression tag	UNP B8LFD6
A	6	GLU	-	expression tag	UNP B8LFD6
A	7	ASP	-	expression tag	UNP B8LFD6
A	8	PRO	-	expression tag	UNP B8LFD6
A	542	ALA	MET	engineered mutation	UNP B8LFD6
B	1	GLY	-	expression tag	UNP B8LFD6
B	2	SER	-	expression tag	UNP B8LFD6
B	3	HIS	-	expression tag	UNP B8LFD6
B	4	MET	-	expression tag	UNP B8LFD6
B	5	LEU	-	expression tag	UNP B8LFD6
B	6	GLU	-	expression tag	UNP B8LFD6
B	7	ASP	-	expression tag	UNP B8LFD6
B	8	PRO	-	expression tag	UNP B8LFD6
B	542	ALA	MET	engineered mutation	UNP B8LFD6
C	1	GLY	-	expression tag	UNP B8LFD6
C	2	SER	-	expression tag	UNP B8LFD6
C	3	HIS	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP B8LFD6
C	5	LEU	-	expression tag	UNP B8LFD6
C	6	GLU	-	expression tag	UNP B8LFD6
C	7	ASP	-	expression tag	UNP B8LFD6
C	8	PRO	-	expression tag	UNP B8LFD6
C	542	ALA	MET	engineered mutation	UNP B8LFD6
D	1	GLY	-	expression tag	UNP B8LFD6
D	2	SER	-	expression tag	UNP B8LFD6
D	3	HIS	-	expression tag	UNP B8LFD6
D	4	MET	-	expression tag	UNP B8LFD6
D	5	LEU	-	expression tag	UNP B8LFD6
D	6	GLU	-	expression tag	UNP B8LFD6
D	7	ASP	-	expression tag	UNP B8LFD6
D	8	PRO	-	expression tag	UNP B8LFD6
D	542	ALA	MET	engineered mutation	UNP B8LFD6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	3	Total Mg 3 3	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		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
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	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	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

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

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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	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	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

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

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

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

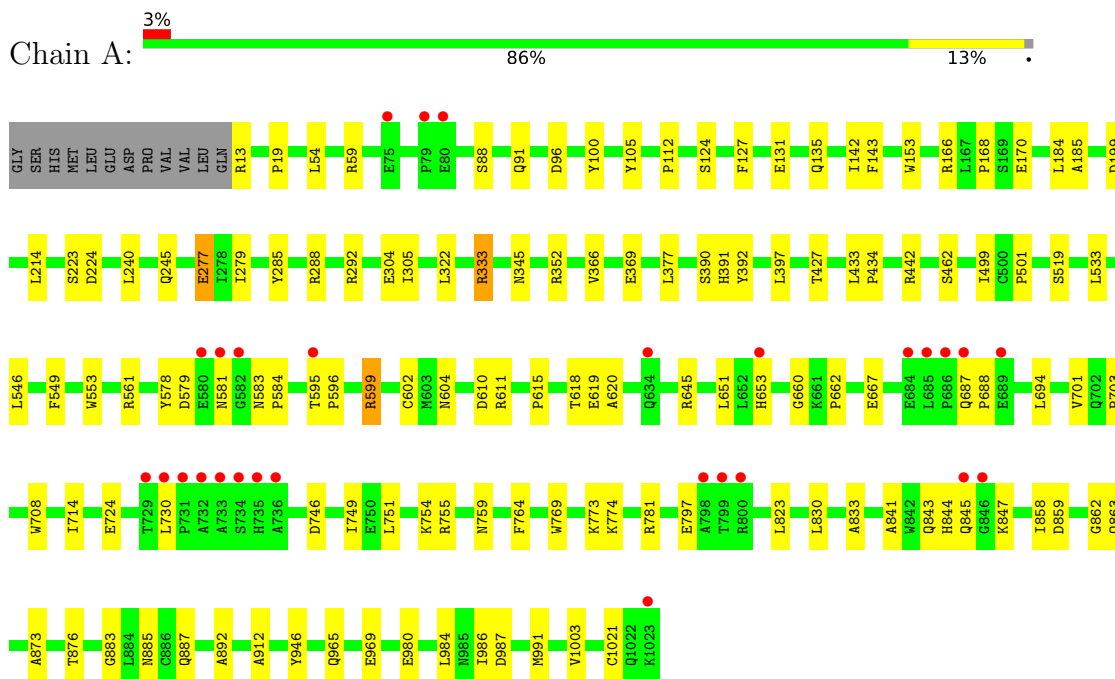
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	941	Total 941	O 941	0	0
5	B	944	Total 944	O 944	0	0
5	C	870	Total 870	O 870	0	0
5	D	856	Total 856	O 856	0	0

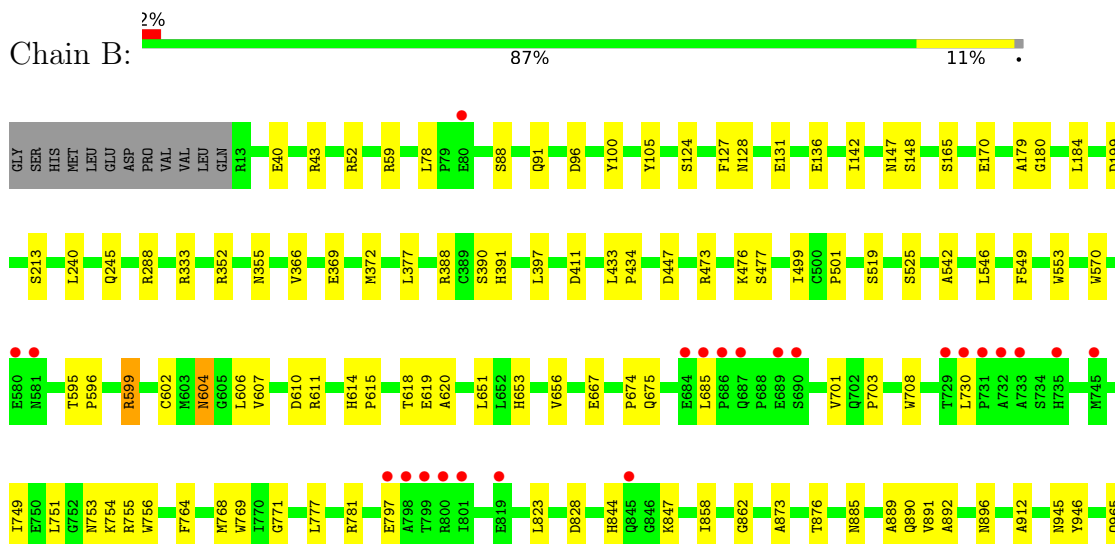
### 3 Residue-property plots i

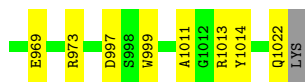
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

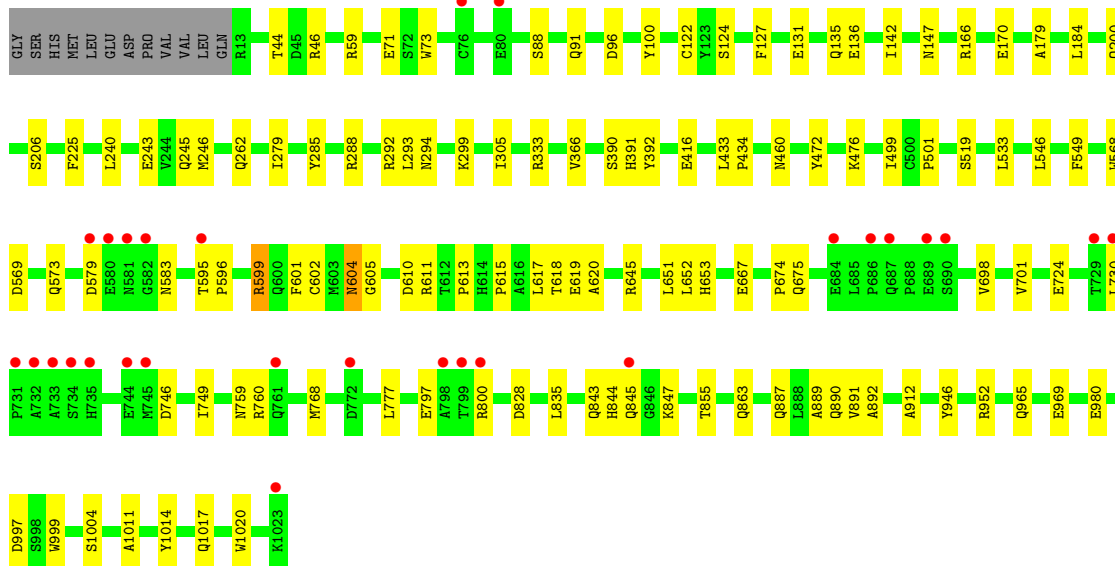
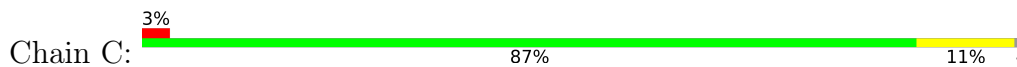


- Molecule 1: Beta-galactosidase

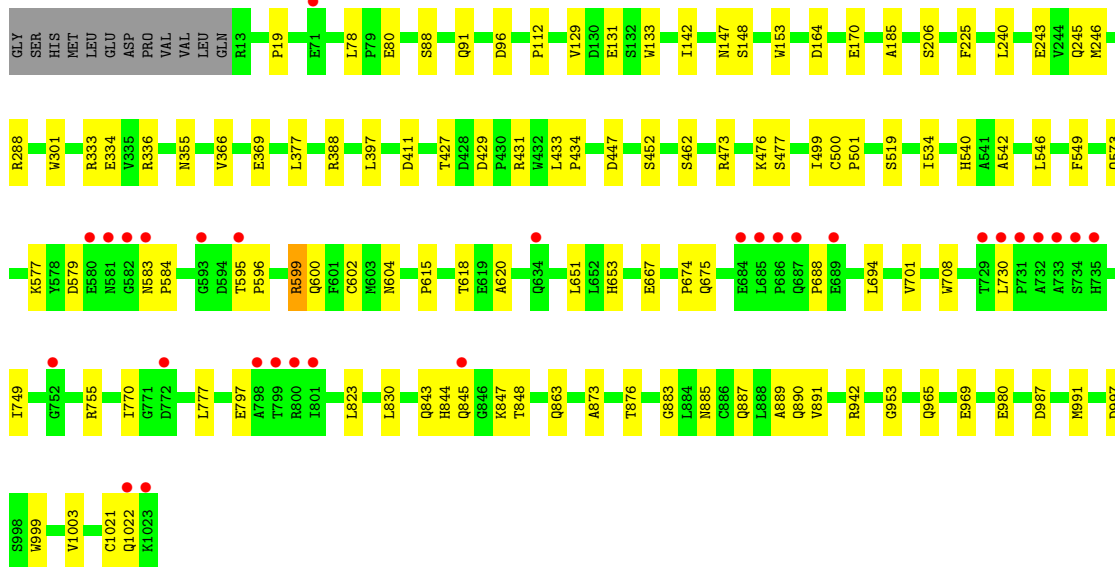
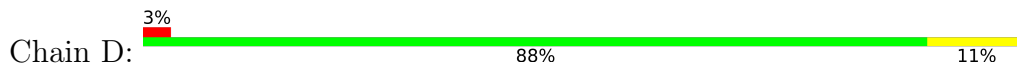




• Molecule 1: Beta-galactosidase



• 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 168.42Å 200.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.70 – 2.10 17.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.70-2.10) 99.9 (17.71-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.11Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.182 , 0.221 0.175 , 0.213	Depositor DCC
$R_{free}$ test set	4227 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	36653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.21 % 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 5.1731e-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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.31	0/8364	0.62	0/11412
1	B	0.32	0/8355	0.62	0/11401
1	C	0.32	0/8364	0.62	0/11412
1	D	0.31	0/8364	0.62	0/11412
All	All	0.32	0/33447	0.62	0/45637

There are no bond length outliers.

There are no bond angle outliers.

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	8122	0	7712	85	0
1	B	8113	0	7699	78	0
1	C	8122	0	7712	78	0
1	D	8122	0	7712	66	0
2	A	5	0	0	0	0
2	B	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	128	0	192	6	0
4	B	136	0	204	2	0
4	C	132	0	198	1	0
4	D	136	0	204	0	0
5	A	941	0	0	3	0
5	B	944	0	0	4	0
5	C	870	0	0	2	0
5	D	856	0	0	2	0
All	All	36653	0	31633	300	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 5.

All (300) 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:C:262:GLN:HE21	1:C:299:LYS:HD3	1.35	0.91
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.63	0.81
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.63	0.81
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.62	0.81
1:C:262:GLN:NE2	1:C:299:LYS:HD3	1.95	0.81
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.66	0.77
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.72	0.72
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.73	0.71
1:D:599:ARG:HH21	1:D:797:GLU:HG3	1.58	0.69
1:C:579:ASP:OD2	1:C:583:ASN:HB2	1.95	0.66
1:D:651:LEU:O	1:D:651:LEU:HD12	1.96	0.66
1:C:88:SER:HA	1:C:366:VAL:HG21	1.77	0.66
1:D:615:PRO:O	1:D:618:THR:HG22	1.97	0.65
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.79	0.65
1:C:965:GLN:O	1:C:969:GLU:HG3	1.97	0.65
1:D:770:ILE:HD13	1:D:1022:GLN:NE2	2.13	0.64
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.13	0.63
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.80	0.63
1:A:751:LEU:HD23	1:A:862:GLY:HA2	1.81	0.62
1:B:88:SER:HA	1:B:366:VAL:HG21	1.81	0.62
1:D:599:ARG:NH2	1:D:797:GLU:HG3	2.14	0.62
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:GLN:HG2	1:B:891:VAL:N	2.14	0.62
1:D:965:GLN:O	1:D:969:GLU:HG3	1.99	0.62
1:A:749:ILE:HD12	1:A:749:ILE:N	2.15	0.62
1:D:88:SER:HA	1:D:366:VAL:HG21	1.82	0.62
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.15	0.61
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.16	0.61
1:A:579:ASP:OD2	1:A:583:ASN:HB2	2.00	0.61
1:C:777:LEU:HG	1:C:889:ALA:HA	1.83	0.60
1:A:304:GLU:HA	5:A:7340:HOH:O	2.02	0.60
1:B:730:LEU:N	1:B:730:LEU:HD12	2.18	0.59
1:A:277:GLU:H	1:A:277:GLU:CD	2.06	0.59
1:D:579:ASP:OD2	1:D:583:ASN:HB2	2.03	0.59
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.01	0.59
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.03	0.58
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.85	0.58
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.86	0.58
1:A:615:PRO:O	1:A:618:THR:HG22	2.03	0.58
1:C:599:ARG:HH21	1:C:797:GLU:CG	2.16	0.58
1:B:165:SER:HB2	5:B:7231:HOH:O	2.04	0.58
1:D:129:VAL:HG12	1:D:133:TRP:HB2	1.86	0.57
1:B:651:LEU:C	1:B:651:LEU:HD12	2.24	0.57
1:C:730:LEU:HD21	1:D:823:LEU:O	2.05	0.57
1:B:651:LEU:HD11	1:B:653:HIS:NE2	2.20	0.57
1:A:131:GLU:O	1:A:135:GLN:HG2	2.05	0.57
1:D:749:ILE:HD12	1:D:749:ILE:N	2.21	0.56
1:B:473:ARG:HH12	1:B:477:SER:HB2	1.71	0.56
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.06	0.56
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.40	0.56
1:B:890:GLN:HG2	1:B:891:VAL:H	1.72	0.55
1:A:730:LEU:HD21	1:B:823:LEU:O	2.05	0.55
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.87	0.55
1:A:887:GLN:NE2	1:A:980:GLU:O	2.36	0.55
1:A:578:TYR:CE1	1:A:584:PRO:HB3	2.41	0.55
1:B:653:HIS:ND1	1:B:667:GLU:HB3	2.22	0.55
1:C:615:PRO:O	1:C:618:THR:HG22	2.05	0.55
1:B:749:ILE:N	1:B:749:ILE:HD12	2.22	0.55
1:B:59:ARG:HB2	1:B:124:SER:OG	2.07	0.55
1:A:88:SER:HA	1:A:366:VAL:HG21	1.89	0.54
1:B:777:LEU:HG	1:B:889:ALA:HA	1.87	0.54
1:A:965:GLN:O	1:A:969:GLU:HG3	2.06	0.54
1:B:599:ARG:HH21	1:B:797:GLU:CG	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASN:H	4:C:8604:DMS:H21	1.72	0.54
1:C:749:ILE:N	1:C:749:ILE:HD12	2.23	0.53
1:A:13:ARG:O	1:A:13:ARG:HG2	2.08	0.53
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.53
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.43	0.53
1:A:581:ASN:HB2	1:A:583:ASN:ND2	2.24	0.53
1:A:833:ALA:HB1	1:A:858:ILE:O	2.08	0.53
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.91	0.53
1:D:129:VAL:CG1	1:D:133:TRP:HB2	2.39	0.53
1:B:844:HIS:O	1:B:847:LYS:HB3	2.09	0.52
1:A:873:ALA:O	1:A:876:THR:HG22	2.08	0.52
1:A:595:THR:HA	1:A:596:PRO:C	2.30	0.52
1:B:973:ARG:HH22	4:B:8609:DMS:H21	1.75	0.52
1:C:136:GLU:HG3	5:C:4754:HOH:O	2.10	0.52
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.08	0.52
1:C:131:GLU:HG3	1:C:135:GLN:HG3	1.90	0.52
1:C:293:LEU:HD12	1:C:293:LEU:N	2.25	0.52
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.52
1:B:599:ARG:NH2	1:B:797:GLU:HG2	2.24	0.52
1:C:651:LEU:HD12	1:C:651:LEU:C	2.30	0.52
1:C:651:LEU:HD11	1:C:653:HIS:NE2	2.25	0.52
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.92	0.52
1:B:610:ASP:O	1:B:611:ARG:HB2	2.08	0.51
1:A:844:HIS:CE1	1:A:845:GLN:HG2	2.45	0.51
1:C:416:GLU:HG3	1:C:460:ASN:O	2.10	0.51
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.46	0.51
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.92	0.51
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.46	0.51
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.75	0.51
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.45	0.51
1:C:147:ASN:HB3	1:C:206:SER:HA	1.92	0.51
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.91	0.51
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.76	0.51
1:C:653:HIS:HD2	1:C:701:VAL:HG21	1.76	0.51
1:A:599:ARG:HH21	1:A:797:GLU:CG	2.23	0.50
1:C:844:HIS:ND1	1:C:845:GLN:HG2	2.25	0.50
1:C:843:GLN:HA	1:C:847:LYS:O	2.12	0.50
1:D:991:MET:HE2	1:D:1003:VAL:HG21	1.92	0.50
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.93	0.50
1:C:240:LEU:C	1:C:240:LEU:HD23	2.32	0.50
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:PRO:O	1:B:675:GLN:HB2	2.12	0.50
1:C:800:ARG:HG2	1:C:800:ARG:HH11	1.77	0.50
1:A:322:LEU:HB2	4:A:8406:DMS:C1	2.41	0.50
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.47	0.50
1:A:653:HIS:ND1	1:A:667:GLU:HB3	2.27	0.49
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.47	0.49
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.93	0.49
1:D:147:ASN:HB3	1:D:206:SER:HA	1.93	0.49
1:B:542:ALA:HA	1:B:604:ASN:HA	1.94	0.49
1:D:577:LYS:O	1:D:584:PRO:HA	2.12	0.49
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.40	0.49
1:B:369:GLU:HA	1:B:372:MET:HE3	1.95	0.49
1:B:372:MET:HE3	1:B:397:LEU:HD23	1.94	0.49
1:A:651:LEU:HD12	1:A:651:LEU:O	2.13	0.49
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.94	0.48
1:C:730:LEU:HD12	1:C:730:LEU:N	2.28	0.48
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.47	0.48
1:C:610:ASP:O	1:C:611:ARG:HB2	2.14	0.48
1:C:292:ARG:C	1:C:293:LEU:HD12	2.33	0.48
1:D:890:GLN:HG2	1:D:891:VAL:N	2.29	0.48
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.96	0.47
1:D:240:LEU:HD23	1:D:240:LEU:C	2.35	0.47
1:D:369:GLU:HG3	1:D:397:LEU:HD21	1.95	0.47
1:D:540:HIS:CE1	1:D:542:ALA:HB2	2.50	0.47
1:A:59:ARG:HB2	1:A:124:SER:OG	2.13	0.47
1:C:279:ILE:HD12	1:C:285:TYR:CD2	2.49	0.47
1:A:730:LEU:HD12	1:A:730:LEU:N	2.30	0.47
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.96	0.47
1:B:651:LEU:HD11	1:B:653:HIS:CD2	2.49	0.47
1:B:873:ALA:O	1:B:876:THR:HG22	2.15	0.47
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.50	0.47
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.96	0.47
1:D:730:LEU:N	1:D:730:LEU:HD12	2.29	0.47
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.97	0.47
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.50	0.47
1:C:599:ARG:HH21	1:C:797:GLU:CD	2.18	0.47
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.96	0.47
1:D:595:THR:HA	1:D:596:PRO:C	2.35	0.47
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.50	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.97	0.47
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HH12	4:A:8412:DMS:H13	1.80	0.46
1:B:599:ARG:NH2	1:B:797:GLU:CG	2.78	0.46
1:C:599:ARG:NH2	1:C:797:GLU:CG	2.78	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.35	0.46
1:A:427:THR:HG21	1:A:462:SER:HB3	1.96	0.46
1:C:568:TRP:HE1	1:C:604:ASN:ND2	2.14	0.46
1:C:569:ASP:O	1:C:605:GLY:HA2	2.15	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.96	0.46
1:A:610:ASP:O	1:A:611:ARG:HB2	2.16	0.46
1:A:688:PRO:HD2	5:A:6031:HOH:O	2.16	0.46
1:B:390:SER:HA	1:B:391:HIS:HA	1.78	0.46
1:C:828:ASP:HB3	1:D:830:LEU:HD22	1.98	0.46
1:D:301:TRP:CH2	1:D:452:SER:HA	2.50	0.46
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.98	0.46
1:A:390:SER:HA	1:A:391:HIS:HA	1.78	0.46
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.98	0.46
1:A:223:SER:O	1:A:224:ASP:HB2	2.16	0.46
1:A:651:LEU:HD12	1:A:651:LEU:C	2.35	0.46
1:C:59:ARG:HB2	1:C:124:SER:OG	2.16	0.46
1:A:599:ARG:NH2	1:A:797:GLU:HG2	2.31	0.46
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.16	0.46
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.51	0.46
1:D:688:PRO:HD3	1:D:694:LEU:HD11	1.98	0.46
1:B:476:LYS:HA	5:B:4204:HOH:O	2.16	0.46
1:D:887:GLN:NE2	1:D:980:GLU:O	2.46	0.46
1:C:651:LEU:HD11	1:C:653:HIS:CD2	2.51	0.45
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.98	0.45
1:B:965:GLN:O	1:B:969:GLU:HG3	2.15	0.45
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.51	0.45
1:C:746:ASP:OD1	1:C:759:ASN:HA	2.16	0.45
1:C:844:HIS:CE1	1:C:845:GLN:HG2	2.51	0.45
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.52	0.45
1:B:599:ARG:HH21	1:B:797:GLU:CD	2.20	0.45
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.16	0.45
1:C:653:HIS:ND1	1:C:667:GLU:HB3	2.31	0.45
1:A:773:LYS:HE2	1:A:774:LYS:O	2.16	0.45
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.52	0.45
1:D:473:ARG:NH1	1:D:477:SER:HB2	2.32	0.45
1:A:714:ILE:HD13	4:A:8603:DMS:H13	1.99	0.45
1:C:1017:GLN:HB2	5:C:6159:HOH:O	2.16	0.45
1:A:54:LEU:HD11	1:A:214:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:O	1:B:213:SER:HB2	2.17	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45
1:D:991:MET:CE	1:D:1003:VAL:HG21	2.45	0.45
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.17	0.44
1:D:225:PHE:HA	1:D:243:GLU:O	2.17	0.44
1:A:292:ARG:HH12	4:A:8412:DMS:C1	2.30	0.44
1:C:863:GLN:OE1	1:C:952:ARG:NH2	2.51	0.44
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.17	0.44
1:B:653:HIS:HD2	1:B:701:VAL:HG21	1.82	0.44
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.53	0.44
1:C:279:ILE:HD12	1:C:285:TYR:CE2	2.53	0.44
1:D:873:ALA:O	1:D:876:THR:HG22	2.18	0.44
1:C:652:LEU:HD11	1:C:698:VAL:HB	2.00	0.44
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.46	0.44
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.44
1:A:764:PHE:CE2	1:A:781:ARG:NH2	2.86	0.44
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.52	0.44
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.48	0.44
1:C:595:THR:HA	1:C:596:PRO:C	2.38	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.18	0.43
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.00	0.43
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.47	0.43
1:A:19:PRO:HD3	1:A:112:PRO:CB	2.49	0.43
1:A:561:ARG:HD3	1:B:525:SER:O	2.19	0.43
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.19	0.43
1:D:942:ARG:HA	1:D:953:GLY:O	2.18	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.43
1:B:896:ASN:HB3	1:B:945:ASN:HB2	2.00	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.99	0.43
1:B:764:PHE:CE2	1:B:781:ARG:NH2	2.87	0.43
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.43
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.53	0.43
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.36	0.43
1:C:166:ARG:HG3	1:C:392:TYR:HB2	2.01	0.43
1:C:599:ARG:NH1	1:C:601:PHE:CZ	2.87	0.43
1:A:701:VAL:O	1:A:703:PRO:HD3	2.18	0.43
1:B:753:ASN:OD1	1:B:771:GLY:HA2	2.18	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.43
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.99	0.43
1:C:568:TRP:NE1	1:C:604:ASN:ND2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:ALA:HB2	1:A:859:ASP:HA	2.01	0.42
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.01	0.42
1:B:997:ASP:HB2	1:B:999:TRP:CZ2	2.54	0.42
1:C:887:GLN:NE2	1:C:980:GLU:O	2.52	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.58	0.42
1:D:843:GLN:HG2	1:D:848:THR:HA	2.01	0.42
1:A:599:ARG:HH21	1:A:797:GLU:HG2	1.84	0.42
1:C:724:GLU:O	1:D:847:LYS:NZ	2.52	0.42
1:A:688:PRO:HD3	1:A:694:LEU:HD11	2.01	0.42
1:B:105:TYR:CE1	1:B:199:ASP:HB2	2.55	0.42
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.54	0.42
1:C:573:GLN:HB2	1:C:602:CYS:O	2.19	0.42
1:D:599:ARG:HB2	1:D:600:GLN:H	1.64	0.42
1:A:687:GLN:CD	1:A:687:GLN:H	2.22	0.42
1:A:823:LEU:HD11	1:A:841:ALA:HB2	2.02	0.42
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.54	0.42
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.40	0.42
1:C:890:GLN:HG2	1:C:891:VAL:N	2.34	0.42
1:D:476:LYS:HD2	5:D:4204:HOH:O	2.19	0.42
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.55	0.42
1:D:651:LEU:HD12	1:D:651:LEU:C	2.40	0.42
1:B:615:PRO:O	1:B:618:THR:HG22	2.20	0.42
1:C:246:MET:SD	1:C:246:MET:C	2.98	0.42
1:A:991:MET:CE	1:A:1003:VAL:HG21	2.50	0.42
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.55	0.42
1:B:973:ARG:HH22	4:B:8609:DMS:C2	2.32	0.42
1:D:246:MET:SD	1:D:246:MET:C	2.99	0.42
1:B:240:LEU:C	1:B:240:LEU:HD23	2.39	0.42
1:B:755:ARG:HD3	5:B:7161:HOH:O	2.19	0.42
1:D:755:ARG:HG3	1:D:755:ARG:HH11	1.85	0.42
1:B:78:LEU:HD23	5:B:4504:HOH:O	2.20	0.41
1:B:606:LEU:O	1:B:614:HIS:HB2	2.20	0.41
1:B:570:TRP:O	1:B:607:VAL:HG22	2.20	0.41
1:B:651:LEU:HD23	1:B:703:PRO:HG3	2.02	0.41
1:B:755:ARG:HB2	1:B:769:TRP:HB2	2.01	0.41
1:B:1013:ARG:HG3	1:B:1013:ARG:HH11	1.85	0.41
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.56	0.41
1:A:660:GLY:O	1:A:662:PRO:HD3	2.20	0.41
1:A:984:LEU:HD21	1:A:986:ILE:HD11	2.02	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:777:LEU:HG	1:D:889:ALA:HA	2.01	0.41
1:A:168:PRO:O	1:A:442:ARG:NH2	2.53	0.41
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.56	0.41
1:A:746:ASP:OD1	1:A:759:ASN:HA	2.20	0.41
1:A:369:GLU:HG3	1:A:397:LEU:HD21	2.02	0.41
1:B:656:VAL:HG21	1:B:685:LEU:HD13	2.03	0.41
1:D:427:THR:HG21	1:D:462:SER:HB3	2.01	0.41
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.51	0.41
1:A:127:PHE:CE2	1:A:214:LEU:HD11	2.55	0.41
1:A:279:ILE:HD12	1:A:285:TYR:CD2	2.56	0.41
1:A:843:GLN:HA	1:A:847:LYS:O	2.20	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.80	0.41
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.56	0.41
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.56	0.41
1:A:724:GLU:O	1:B:847:LYS:NZ	2.53	0.41
1:B:754:LYS:HE3	1:B:1022:GLN:HG3	2.03	0.41
1:C:844:HIS:O	1:C:847:LYS:HB3	2.21	0.41
1:A:322:LEU:HB2	4:A:8406:DMS:H12	2.02	0.41
1:A:533:LEU:C	1:A:533:LEU:HD23	2.41	0.41
1:A:754:LYS:HE2	5:A:4766:HOH:O	2.21	0.41
1:D:674:PRO:O	1:D:675:GLN:HB2	2.21	0.41
1:A:143:PHE:O	1:A:168:PRO:HA	2.21	0.40
1:C:674:PRO:O	1:C:675:GLN:HB2	2.21	0.40
1:D:500:CYS:HA	1:D:534:ILE:O	2.21	0.40
1:A:277:GLU:CD	1:A:277:GLU:N	2.74	0.40
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.56	0.40
1:C:472:TYR:O	1:C:476:LYS:HG2	2.21	0.40
1:A:322:LEU:HB2	4:A:8406:DMS:H13	2.02	0.40
1:A:333:ARG:HA	1:A:345:ASN:OD1	2.21	0.40
1:D:78:LEU:HD23	5:D:4504:HOH:O	2.20	0.40
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.39	0.40
1:D:573:GLN:HB2	1:D:602:CYS:O	2.22	0.40

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	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	51	54
1	B	1008/1023 (98%)	969 (96%)	38 (4%)	1 (0%)	51	54
1	C	1009/1023 (99%)	968 (96%)	40 (4%)	1 (0%)	51	54
1	D	1009/1023 (99%)	961 (95%)	46 (5%)	2 (0%)	47	49
All	All	4035/4092 (99%)	3868 (96%)	162 (4%)	5 (0%)	51	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	599	ARG
1	A	599	ARG
1	B	599	ARG
1	C	599	ARG
1	D	164	ASP

### 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	863/874 (99%)	857 (99%)	6 (1%)	84	88
1	B	862/874 (99%)	855 (99%)	7 (1%)	81	86
1	C	863/874 (99%)	857 (99%)	6 (1%)	84	88
1	D	863/874 (99%)	856 (99%)	7 (1%)	81	86
All	All	3451/3496 (99%)	3425 (99%)	26 (1%)	81	86

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	333	ARG
1	A	519	SER
1	A	546	LEU
1	A	604	ASN
1	A	885	ASN
1	B	136	GLU
1	B	333	ARG
1	B	519	SER
1	B	546	LEU
1	B	604	ASN
1	B	768	MET
1	B	885	ASN
1	C	71	GLU
1	C	333	ARG
1	C	519	SER
1	C	546	LEU
1	C	604	ASN
1	C	1004	SER
1	D	80	GLU
1	D	131	GLU
1	D	333	ARG
1	D	519	SER
1	D	546	LEU
1	D	604	ASN
1	D	885	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	262	GLN
1	A	583	ASN
1	A	757	GLN
1	A	1022	GLN
1	B	554	GLN
1	B	583	ASN
1	B	804	ASN
1	B	863	GLN
1	C	163	GLN
1	D	163	GLN
1	D	583	ASN
1	D	653	HIS
1	D	757	GLN

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Mol	Chain	Res	Type
1	D	804	ASN
1	D	1022	GLN

### 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 164 ligands modelled in this entry, 31 are monoatomic - leaving 133 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	B	8411	-	3,3,3	0.28	0	3,3,3	0.62	0
4	DMS	D	8427	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	D	8407	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	A	8419	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	C	8411	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	D	8413	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	B	8408	-	3,3,3	0.25	0	3,3,3	0.63	0
4	DMS	B	8425	3	3,3,3	0.26	0	3,3,3	0.62	0
4	DMS	A	8414	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	A	8502	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	B	8609	-	3,3,3	0.21	0	3,3,3	0.62	0
4	DMS	C	8602	-	3,3,3	0.23	0	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	D	8423	-	3,3,3	0.24	0	3,3,3	0.60	0
4	DMS	B	8416	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8411	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	A	8401	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	A	8425	3	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	B	8606	-	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	C	8607	-	3,3,3	0.20	0	3,3,3	0.63	0
4	DMS	D	8711	-	3,3,3	0.24	0	3,3,3	0.62	0
4	DMS	C	8408	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	C	8606	-	3,3,3	0.19	0	3,3,3	0.61	0
4	DMS	C	8410	-	3,3,3	0.26	0	3,3,3	0.60	0
4	DMS	B	8409	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	A	8612	-	3,3,3	0.22	0	3,3,3	0.63	0
4	DMS	D	8705	-	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	B	8406	-	3,3,3	0.27	0	3,3,3	0.60	0
4	DMS	B	8607	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8607	-	3,3,3	0.23	0	3,3,3	0.62	0
4	DMS	C	8414	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	C	8421	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	B	8601	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	C	8415	-	3,3,3	0.23	0	3,3,3	0.62	0
4	DMS	C	1024	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	B	8508	-	3,3,3	0.25	0	3,3,3	0.64	0
4	DMS	C	8503	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	B	8407	-	3,3,3	0.23	0	3,3,3	0.62	0
4	DMS	D	8405	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	C	8412	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	A	8420	-	3,3,3	0.22	0	3,3,3	0.62	0
4	DMS	A	8409	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	C	8401	-	3,3,3	0.21	0	3,3,3	0.65	0
4	DMS	A	8406	-	3,3,3	0.20	0	3,3,3	0.51	0
4	DMS	C	8425	3	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	D	8709	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	B	8604	-	3,3,3	0.25	0	3,3,3	0.64	0
4	DMS	D	8707	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	A	8604	-	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	D	8403	-	3,3,3	0.21	0	3,3,3	0.61	0
4	DMS	A	8427	-	3,3,3	0.24	0	3,3,3	0.64	0
4	DMS	D	8421	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	B	8412	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	A	8407	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	D	8404	-	3,3,3	0.22	0	3,3,3	0.62	0
4	DMS	C	8601	-	3,3,3	0.25	0	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	B	8502	-	3,3,3	0.26	0	3,3,3	0.65	0
4	DMS	B	8417	-	3,3,3	0.24	0	3,3,3	0.64	0
4	DMS	A	8412	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	A	8403	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	C	8409	-	3,3,3	0.21	0	3,3,3	0.61	0
4	DMS	D	8712	-	3,3,3	0.20	0	3,3,3	0.61	0
4	DMS	D	8416	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	A	8413	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8405	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	B	8608	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	D	8411	-	3,3,3	0.24	0	3,3,3	0.62	0
4	DMS	A	8610	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	A	8609	-	3,3,3	0.25	0	3,3,3	0.64	0
4	DMS	C	8427	-	3,3,3	0.21	0	3,3,3	0.61	0
4	DMS	C	8407	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	B	8405	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	B	8610	-	3,3,3	0.20	0	3,3,3	0.63	0
4	DMS	B	8605	-	3,3,3	0.22	0	3,3,3	0.63	0
4	DMS	C	8604	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	D	8701	-	3,3,3	0.27	0	3,3,3	0.58	0
4	DMS	D	8710	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	B	8410	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	B	8603	-	3,3,3	0.16	0	3,3,3	0.63	0
4	DMS	A	8410	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	A	8504	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	B	8423	-	3,3,3	0.24	0	3,3,3	0.59	0
4	DMS	D	8410	-	3,3,3	0.24	0	3,3,3	0.60	0
4	DMS	B	8404	-	3,3,3	0.19	0	3,3,3	0.60	0
4	DMS	C	8603	-	3,3,3	0.26	0	3,3,3	0.60	0
4	DMS	A	8605	-	3,3,3	0.24	0	3,3,3	0.57	0
4	DMS	D	8408	-	3,3,3	0.28	0	3,3,3	0.63	0
4	DMS	B	8504	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	A	8603	-	3,3,3	0.25	0	3,3,3	0.61	0
4	DMS	C	8417	-	3,3,3	0.23	0	3,3,3	0.63	0
4	DMS	A	8404	-	3,3,3	0.21	0	3,3,3	0.61	0
4	DMS	D	8414	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	C	8416	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	B	8414	-	3,3,3	0.24	0	3,3,3	0.60	0
4	DMS	D	8415	-	3,3,3	0.21	0	3,3,3	0.62	0
4	DMS	A	8503	-	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	A	8421	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	B	8421	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	D	8503	-	3,3,3	0.21	0	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	D	8706	-	3,3,3	0.26	0	3,3,3	0.63	0
4	DMS	B	8401	-	3,3,3	0.23	0	3,3,3	0.63	0
4	DMS	D	8412	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	D	8419	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	C	8504	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	D	8401	-	3,3,3	0.22	0	3,3,3	0.63	0
4	DMS	D	8425	3	3,3,3	0.27	0	3,3,3	0.62	0
4	DMS	C	8419	-	3,3,3	0.25	0	3,3,3	0.62	0
4	DMS	C	8402	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	C	8405	-	3,3,3	0.20	0	3,3,3	0.59	0
4	DMS	B	8402	-	3,3,3	0.19	0	3,3,3	0.55	0
4	DMS	B	8413	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	C	8413	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	D	8501	-	3,3,3	0.24	0	3,3,3	0.62	0
4	DMS	A	8408	-	3,3,3	0.24	0	3,3,3	0.64	0
4	DMS	D	8402	-	3,3,3	0.18	0	3,3,3	0.57	0
4	DMS	C	8501	-	3,3,3	0.19	0	3,3,3	0.59	0
4	DMS	C	8420	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	D	8406	-	3,3,3	0.27	0	3,3,3	0.60	0
4	DMS	C	8423	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	B	8403	-	3,3,3	0.23	0	3,3,3	0.63	0
4	DMS	D	8508	-	3,3,3	0.23	0	3,3,3	0.63	0
4	DMS	C	8404	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	A	8402	-	3,3,3	0.23	0	3,3,3	0.56	0
4	DMS	A	8602	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8608	-	3,3,3	0.21	0	3,3,3	0.63	0
4	DMS	C	8403	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	A	8501	-	3,3,3	0.20	0	3,3,3	0.61	0
4	DMS	B	8415	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	D	8703	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	B	8602	-	3,3,3	0.22	0	3,3,3	0.61	0
4	DMS	C	8605	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	D	8708	-	3,3,3	0.23	0	3,3,3	0.62	0
4	DMS	D	8409	-	3,3,3	0.21	0	3,3,3	0.59	0
4	DMS	B	8427	-	3,3,3	0.22	0	3,3,3	0.62	0

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.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8609	DMS	2	0
4	A	8406	DMS	3	0
4	A	8412	DMS	2	0
4	C	8604	DMS	1	0
4	A	8603	DMS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1011/1023 (98%)	-0.32	28 (2%) 53 59	5, 15, 33, 68	0
1	B	1010/1023 (98%)	-0.36	23 (2%) 60 65	4, 15, 31, 65	0
1	C	1011/1023 (98%)	-0.37	28 (2%) 53 59	5, 14, 33, 61	0
1	D	1011/1023 (98%)	-0.32	29 (2%) 51 57	5, 16, 34, 69	0
All	All	4043/4092 (98%)	-0.34	108 (2%) 54 60	4, 15, 33, 69	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	9.3
1	A	735	HIS	8.8
1	C	731	PRO	8.7
1	B	731	PRO	8.3
1	A	686	PRO	8.0
1	D	732	ALA	8.0
1	D	735	HIS	7.3
1	C	732	ALA	7.2
1	A	730	LEU	6.8
1	D	689	GLU	6.5
1	D	730	LEU	6.3
1	D	731	PRO	6.2
1	B	689	GLU	6.1
1	C	689	GLU	6.0
1	C	730	LEU	5.9
1	D	581	ASN	5.8
1	C	735	HIS	5.7
1	A	731	PRO	5.5
1	D	798	ALA	5.4
1	D	684	GLU	5.3
1	A	732	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	580	GLU	5.2
1	A	1023	LYS	5.2
1	B	730	LEU	5.1
1	C	798	ALA	5.1
1	B	687	GLN	5.1
1	B	684	GLU	5.1
1	D	687	GLN	5.0
1	A	689	GLU	5.0
1	D	799	THR	5.0
1	A	800	ARG	4.9
1	D	800	ARG	4.9
1	C	580	GLU	4.6
1	C	772	ASP	4.4
1	A	733	ALA	4.4
1	D	734	SER	4.3
1	D	686	PRO	4.3
1	A	687	GLN	4.3
1	D	685	LEU	4.2
1	B	686	PRO	4.2
1	C	800	ARG	4.1
1	B	797	GLU	4.1
1	B	580	GLU	4.1
1	A	798	ALA	4.1
1	A	734	SER	4.0
1	B	733	ALA	4.0
1	D	733	ALA	4.0
1	B	798	ALA	3.9
1	A	580	GLU	3.8
1	A	729	THR	3.8
1	A	799	THR	3.7
1	C	733	ALA	3.7
1	A	684	GLU	3.6
1	D	595	THR	3.6
1	B	800	ARG	3.5
1	C	684	GLU	3.4
1	D	772	ASP	3.4
1	C	687	GLN	3.3
1	A	581	ASN	3.3
1	D	71	GLU	3.2
1	B	735	HIS	3.2
1	B	729	THR	3.1
1	A	736	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	845	GLN	3.0
1	B	581	ASN	2.9
1	C	595	THR	2.9
1	C	799	THR	2.9
1	A	846	GLY	2.8
1	B	799	THR	2.7
1	C	729	THR	2.7
1	C	745	MET	2.7
1	A	685	LEU	2.6
1	C	686	PRO	2.6
1	B	685	LEU	2.6
1	A	634	GLN	2.5
1	B	819	GLU	2.4
1	D	583	ASN	2.4
1	C	690	SER	2.4
1	B	745	MET	2.4
1	C	744	GLU	2.4
1	D	845	GLN	2.4
1	D	1022	GLN	2.4
1	C	582	GLY	2.4
1	A	80	GLU	2.3
1	D	582	GLY	2.3
1	C	1023	LYS	2.3
1	A	582	GLY	2.3
1	D	1023	LYS	2.3
1	D	801	ILE	2.3
1	C	734	SER	2.3
1	B	80	GLU	2.3
1	C	76	CYS	2.2
1	B	690	SER	2.2
1	D	593	GLY	2.2
1	A	653	HIS	2.2
1	A	595	THR	2.2
1	C	581	ASN	2.1
1	C	579	ASP	2.1
1	A	75	GLU	2.1
1	D	752	GLY	2.1
1	C	80	GLU	2.1
1	D	729	THR	2.1
1	A	845	GLN	2.1
1	B	845	GLN	2.1
1	D	634	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	801	ILE	2.1
1	A	79	PRO	2.0
1	C	761	GLN	2.0

## 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(Å <sup>2</sup> )	Q<0.9
4	DMS	B	8609	4/4	0.27	0.39	74,75,75,76	0
4	DMS	A	8413	4/4	0.64	0.35	99,99,99,99	0
4	DMS	D	8407	4/4	0.72	0.32	49,50,51,51	0
4	DMS	B	8413	4/4	0.75	0.29	64,65,65,66	0
4	DMS	B	8610	4/4	0.76	0.21	67,67,67,68	0
4	DMS	D	8413	4/4	0.76	0.41	83,84,84,84	0
4	DMS	A	8502	4/4	0.78	0.30	51,53,53,54	0
4	DMS	C	8415	4/4	0.78	0.27	53,55,55,56	0
4	DMS	D	8705	4/4	0.78	0.22	60,61,62,63	0
4	DMS	D	8415	4/4	0.80	0.27	59,59,59,61	0
4	DMS	B	8608	4/4	0.81	0.29	75,75,75,75	0
4	DMS	D	8708	4/4	0.81	0.23	72,72,73,73	0
4	DMS	A	8427	4/4	0.83	0.24	84,84,84,84	0
2	MG	C	3003	1/1	0.83	0.14	24,24,24,24	1
2	MG	A	3003	1/1	0.83	0.23	56,56,56,56	0
3	NA	C	3101	1/1	0.85	0.09	35,35,35,35	0
4	DMS	A	8414	4/4	0.85	0.22	60,61,61,61	0
4	DMS	C	8413	4/4	0.85	0.25	79,79,79,79	0
4	DMS	A	8410	4/4	0.85	0.21	54,54,55,55	0
4	DMS	C	8602	4/4	0.85	0.19	64,64,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	D	8710	4/4	0.85	0.20	60,60,60,60	0
4	DMS	B	8406	4/4	0.86	0.27	74,74,74,74	0
4	DMS	A	8605	4/4	0.86	0.36	49,50,51,51	0
4	DMS	B	8603	4/4	0.86	0.18	41,42,44,44	0
4	DMS	D	8711	4/4	0.86	0.22	49,50,51,51	0
4	DMS	A	8604	4/4	0.87	0.27	74,75,75,75	0
4	DMS	B	8508	4/4	0.87	0.23	53,54,54,55	0
4	DMS	B	8410	4/4	0.88	0.14	73,73,74,74	0
4	DMS	D	8414	4/4	0.88	0.23	49,50,50,51	0
2	MG	D	3003	1/1	0.88	0.23	48,48,48,48	0
4	DMS	C	8601	4/4	0.88	0.23	45,45,46,47	0
4	DMS	D	8706	4/4	0.88	0.19	54,54,54,55	0
4	DMS	B	8415	4/4	0.88	0.22	63,63,64,64	0
4	DMS	D	8404	4/4	0.88	0.17	46,47,47,48	0
2	MG	B	3003	1/1	0.88	0.16	38,38,38,38	0
4	DMS	D	8712	4/4	0.88	0.22	67,67,67,68	0
4	DMS	A	8407	4/4	0.89	0.26	48,48,48,49	0
4	DMS	D	8421	4/4	0.89	0.21	67,67,67,67	0
4	DMS	B	8602	4/4	0.89	0.13	46,47,48,49	0
4	DMS	A	8406	4/4	0.89	0.22	42,45,46,47	0
4	DMS	A	8607	4/4	0.89	0.16	71,71,71,71	0
4	DMS	A	8610	4/4	0.89	0.15	44,45,45,46	0
4	DMS	B	8417	4/4	0.89	0.18	54,54,55,56	0
4	DMS	B	8423	4/4	0.89	0.20	70,70,71,71	0
4	DMS	A	8609	4/4	0.90	0.13	58,58,58,60	0
4	DMS	B	8604	4/4	0.90	0.20	55,55,56,56	0
4	DMS	C	8423	4/4	0.90	0.14	63,63,63,63	0
4	DMS	B	8605	4/4	0.90	0.22	55,55,56,56	0
4	DMS	C	8407	4/4	0.90	0.22	63,64,64,64	0
4	DMS	C	8607	4/4	0.90	0.13	37,37,38,41	0
4	DMS	D	8423	4/4	0.91	0.18	55,55,55,55	0
4	DMS	D	8427	4/4	0.91	0.25	69,69,69,70	0
4	DMS	D	8703	4/4	0.91	0.22	63,63,63,64	0
3	NA	A	3101	1/1	0.91	0.06	36,36,36,36	0
4	DMS	C	8420	4/4	0.91	0.16	56,57,57,57	0
4	DMS	B	8404	4/4	0.91	0.12	30,31,34,34	0
4	DMS	A	8602	4/4	0.91	0.23	65,65,65,65	0
4	DMS	D	8416	4/4	0.91	0.21	47,48,49,50	0
4	DMS	B	8407	4/4	0.91	0.21	56,56,56,57	0
2	MG	A	3005	1/1	0.92	0.06	40,40,40,40	0
4	DMS	C	8503	4/4	0.92	0.24	64,64,64,65	0
4	DMS	C	8504	4/4	0.92	0.17	48,48,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	B	8607	4/4	0.92	0.18	69,69,69,70	0
4	DMS	D	8707	4/4	0.92	0.14	53,54,54,54	0
4	DMS	B	8427	4/4	0.92	0.20	52,53,53,54	0
4	DMS	C	8416	4/4	0.92	0.26	53,53,54,54	0
4	DMS	C	1024	4/4	0.92	0.15	60,60,60,61	0
4	DMS	D	8425	4/4	0.92	0.22	36,36,36,36	4
4	DMS	C	8604	4/4	0.93	0.19	57,57,58,58	0
4	DMS	C	8605	4/4	0.93	0.23	54,54,55,55	0
4	DMS	A	8421	4/4	0.93	0.26	56,56,56,57	0
4	DMS	D	8501	4/4	0.93	0.14	52,52,53,54	0
4	DMS	A	8404	4/4	0.93	0.11	40,41,42,43	0
4	DMS	D	8406	4/4	0.93	0.15	34,34,35,36	0
4	DMS	B	8416	4/4	0.93	0.19	57,57,58,58	0
4	DMS	C	8501	4/4	0.93	0.12	38,39,40,40	0
3	NA	B	3101	1/1	0.93	0.04	26,26,26,26	0
4	DMS	A	8608	4/4	0.93	0.16	51,52,52,52	0
4	DMS	B	8606	4/4	0.93	0.21	59,60,60,60	0
2	MG	C	3006	1/1	0.93	0.05	37,37,37,37	0
4	DMS	B	8502	4/4	0.94	0.20	33,33,34,35	0
4	DMS	A	8603	4/4	0.94	0.31	80,80,80,80	0
3	NA	D	3101	1/1	0.94	0.07	36,36,36,36	0
4	DMS	C	8404	4/4	0.94	0.13	37,37,37,38	0
4	DMS	A	8612	4/4	0.94	0.14	63,63,63,63	0
4	DMS	C	8410	4/4	0.94	0.21	48,48,49,49	0
4	DMS	D	8508	4/4	0.94	0.16	56,56,57,57	0
4	DMS	A	8420	4/4	0.94	0.13	53,53,53,54	0
4	DMS	A	8503	4/4	0.94	0.34	58,58,58,59	0
2	MG	A	3009	1/1	0.94	0.07	43,43,43,43	0
4	DMS	C	8417	4/4	0.94	0.15	55,55,55,55	0
4	DMS	C	8419	4/4	0.94	0.11	75,75,76,76	0
4	DMS	B	8425	4/4	0.94	0.22	48,49,49,49	0
4	DMS	B	8409	4/4	0.94	0.16	35,35,36,36	0
4	DMS	C	8425	4/4	0.94	0.29	46,47,47,47	0
4	DMS	C	8411	4/4	0.95	0.13	36,38,39,39	0
4	DMS	D	8419	4/4	0.95	0.14	62,62,63,63	0
4	DMS	B	8411	4/4	0.95	0.15	36,37,38,39	0
4	DMS	A	8408	4/4	0.95	0.17	39,39,40,41	0
4	DMS	C	8603	4/4	0.95	0.17	47,47,47,47	0
4	DMS	B	8504	4/4	0.95	0.14	46,47,47,48	0
4	DMS	A	8501	4/4	0.95	0.12	37,37,38,39	0
4	DMS	D	8503	4/4	0.95	0.17	53,53,54,54	0
4	DMS	C	8606	4/4	0.95	0.12	47,48,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	B	8601	4/4	0.95	0.17	50,50,50,50	0
4	DMS	A	8419	4/4	0.95	0.22	70,70,70,70	0
3	NA	D	3104	1/1	0.95	0.06	30,30,30,30	0
3	NA	B	3104	1/1	0.95	0.09	28,28,28,28	0
4	DMS	D	8409	4/4	0.95	0.17	40,40,41,41	0
4	DMS	C	8427	4/4	0.95	0.17	52,52,52,52	0
4	DMS	C	8409	4/4	0.95	0.15	39,40,40,41	0
4	DMS	A	8425	4/4	0.95	0.17	45,45,46,46	0
4	DMS	C	8421	4/4	0.96	0.17	51,51,51,51	0
2	MG	A	3001	1/1	0.96	0.04	17,17,17,17	0
3	NA	B	3103	1/1	0.96	0.08	30,30,30,30	0
4	DMS	B	8421	4/4	0.96	0.10	57,57,57,58	0
3	NA	C	3104	1/1	0.96	0.12	26,26,26,26	0
4	DMS	A	8504	4/4	0.96	0.10	47,47,47,47	0
4	DMS	D	8701	4/4	0.96	0.12	29,29,29,30	0
4	DMS	D	8410	4/4	0.96	0.19	42,43,43,44	0
4	DMS	D	8411	4/4	0.96	0.12	36,37,39,39	0
4	DMS	C	8414	4/4	0.96	0.19	42,43,43,43	0
4	DMS	B	8405	4/4	0.96	0.16	35,35,36,36	0
4	DMS	C	8402	4/4	0.96	0.09	19,20,23,24	0
4	DMS	D	8709	4/4	0.96	0.17	69,70,70,70	0
4	DMS	C	8403	4/4	0.96	0.12	27,28,28,30	0
4	DMS	A	8409	4/4	0.96	0.18	43,43,43,44	0
4	DMS	C	8405	4/4	0.96	0.12	30,31,32,32	0
4	DMS	B	8408	4/4	0.97	0.18	30,31,31,31	0
3	NA	C	3103	1/1	0.97	0.09	28,28,28,28	0
4	DMS	C	8401	4/4	0.97	0.09	14,17,20,21	0
4	DMS	A	8405	4/4	0.97	0.09	23,24,25,26	0
4	DMS	D	8401	4/4	0.97	0.09	16,17,21,22	0
4	DMS	D	8402	4/4	0.97	0.08	16,17,17,19	0
2	MG	B	3001	1/1	0.97	0.05	14,14,14,14	0
4	DMS	D	8405	4/4	0.97	0.11	29,29,29,29	0
4	DMS	B	8412	4/4	0.97	0.10	31,32,32,34	0
2	MG	D	3001	1/1	0.97	0.04	16,16,16,16	0
4	DMS	D	8408	4/4	0.97	0.15	34,34,35,36	0
4	DMS	B	8414	4/4	0.97	0.15	46,46,47,47	0
4	DMS	B	8402	4/4	0.97	0.09	15,18,18,20	0
4	DMS	B	8403	4/4	0.97	0.09	28,29,29,30	0
3	NA	C	3102	1/1	0.97	0.05	9,9,9,9	0
4	DMS	A	8402	4/4	0.97	0.11	21,21,22,24	0
4	DMS	A	8403	4/4	0.97	0.10	31,32,33,34	0
4	DMS	A	8412	4/4	0.97	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	D	3103	1/1	0.98	0.07	31,31,31,31	0
2	MG	C	3001	1/1	0.98	0.05	14,14,14,14	0
4	DMS	A	8401	4/4	0.98	0.10	18,18,20,21	0
4	DMS	A	8411	4/4	0.98	0.09	44,44,44,45	0
3	NA	A	3102	1/1	0.98	0.06	9,9,9,9	0
4	DMS	D	8412	4/4	0.98	0.14	34,35,36,36	0
4	DMS	C	8408	4/4	0.98	0.09	33,34,34,35	0
3	NA	A	3103	1/1	0.98	0.07	29,29,29,29	0
3	NA	A	3104	1/1	0.98	0.07	28,28,28,28	0
2	MG	C	3002	1/1	0.98	0.05	13,13,13,13	0
4	DMS	D	8403	4/4	0.98	0.08	31,31,32,33	0
4	DMS	C	8412	4/4	0.98	0.10	38,38,39,39	0
2	MG	B	3002	1/1	0.98	0.03	11,11,11,11	0
3	NA	D	3102	1/1	0.98	0.06	9,9,9,9	0
2	MG	A	3002	1/1	0.99	0.06	15,15,15,15	0
2	MG	D	3002	1/1	0.99	0.05	14,14,14,14	0
3	NA	B	3102	1/1	0.99	0.03	12,12,12,12	0
4	DMS	B	8401	4/4	0.99	0.06	12,16,19,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.