wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2023 – 11:15 PM EDT

PDB ID	:	4TTG
Title	:	Beta-galactosidase (E. coli) in the presence of potassium chloride.
Authors	:	Juers, D.H.
Deposited on	:	2014-06-20
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

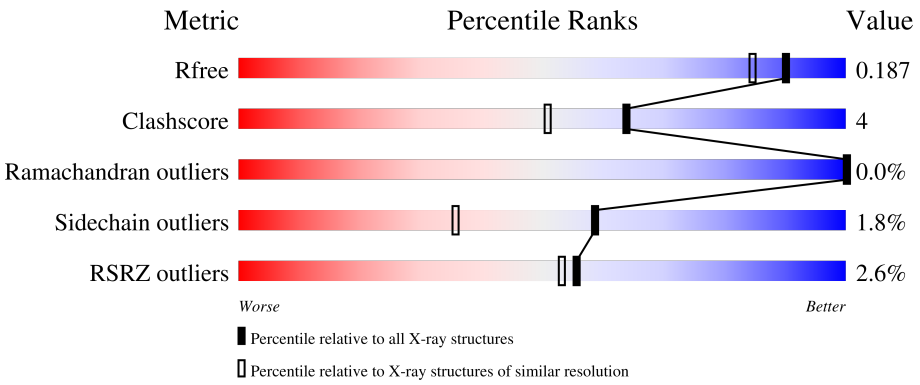
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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 >=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 <=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% 88% 10% ••
1	B	1023	2% 89% 10% ••
1	C	1023	2% 88% 10% ••
1	D	1023	3% 89% 9% ••

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
5	DMS	A	3023	-	-	X	-
5	DMS	A	3025	-	-	X	-
5	DMS	B	1119	-	-	X	-
5	DMS	B	1122	-	-	X	-
5	DMS	B	1127	-	-	X	-
5	DMS	C	3019	-	-	X	-
5	DMS	C	3029	-	-	X	-
5	DMS	C	3034	-	-	X	-
5	DMS	D	1122	-	-	X	-
5	DMS	D	1129	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 38364 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	1015	8365	5304	1475	1542	44	0	35	0
1	B	1015	8315	5272	1463	1537	43	0	29	0
1	C	1015	8342	5286	1471	1542	43	0	31	0
1	D	1015	8328	5284	1462	1538	44	0	33	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8VNN2
A	2	SER	-	expression tag	UNP Q8VNN2
A	3	HIS	-	expression tag	UNP Q8VNN2
A	4	MET	-	expression tag	UNP Q8VNN2
A	5	LEU	-	expression tag	UNP Q8VNN2
A	6	GLU	-	expression tag	UNP Q8VNN2
A	7	ASP	-	expression tag	UNP Q8VNN2
A	8	PRO	-	expression tag	UNP Q8VNN2
B	1	GLY	-	expression tag	UNP Q8VNN2
B	2	SER	-	expression tag	UNP Q8VNN2
B	3	HIS	-	expression tag	UNP Q8VNN2
B	4	MET	-	expression tag	UNP Q8VNN2
B	5	LEU	-	expression tag	UNP Q8VNN2
B	6	GLU	-	expression tag	UNP Q8VNN2
B	7	ASP	-	expression tag	UNP Q8VNN2
B	8	PRO	-	expression tag	UNP Q8VNN2
C	1	GLY	-	expression tag	UNP Q8VNN2
C	2	SER	-	expression tag	UNP Q8VNN2
C	3	HIS	-	expression tag	UNP Q8VNN2
C	4	MET	-	expression tag	UNP Q8VNN2
C	5	LEU	-	expression tag	UNP Q8VNN2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	-	expression tag	UNP Q8VNN2
C	7	ASP	-	expression tag	UNP Q8VNN2
C	8	PRO	-	expression tag	UNP Q8VNN2
D	1	GLY	-	expression tag	UNP Q8VNN2
D	2	SER	-	expression tag	UNP Q8VNN2
D	3	HIS	-	expression tag	UNP Q8VNN2
D	4	MET	-	expression tag	UNP Q8VNN2
D	5	LEU	-	expression tag	UNP Q8VNN2
D	6	GLU	-	expression tag	UNP Q8VNN2
D	7	ASP	-	expression tag	UNP Q8VNN2
D	8	PRO	-	expression tag	UNP Q8VNN2

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

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

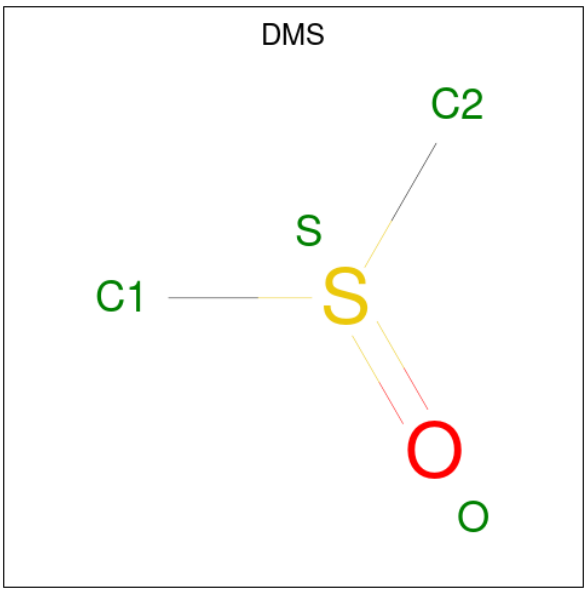
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	8	4	2	2	0	1
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0
			Total	C	O	S		
5	D	1	4	2	1	1	0	0

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

- Molecule 6 is water.

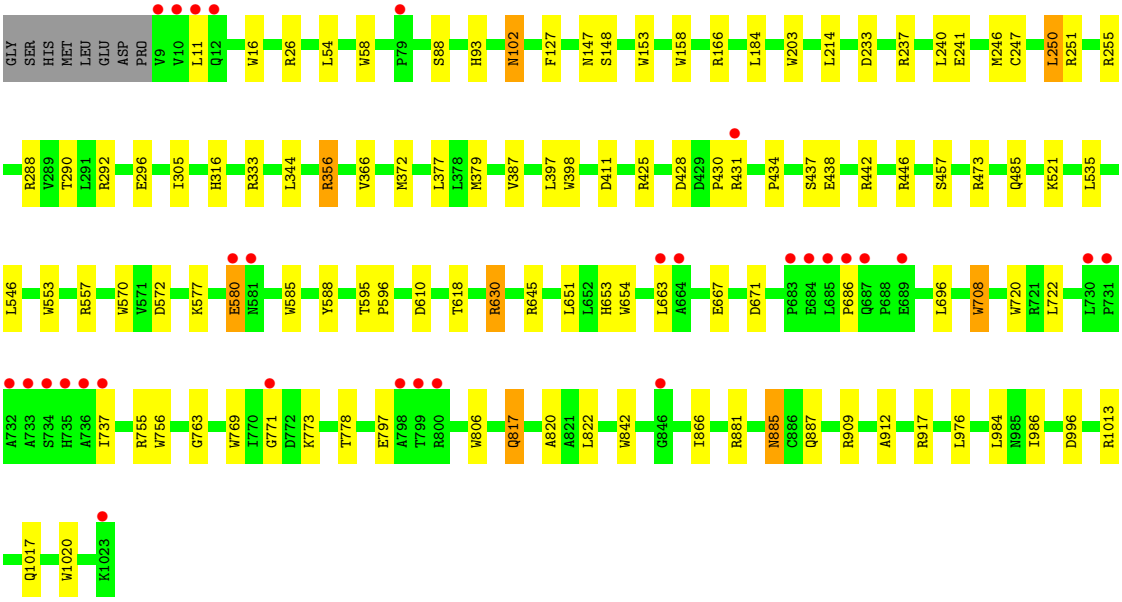
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	1130	1130	1130	0	0
			Total	O		
6	B	1114	1114	1114	0	0
			Total	O		
6	C	1094	1094	1094	0	0
			Total	O		
6	D	1113	1113	1113	0	0

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.

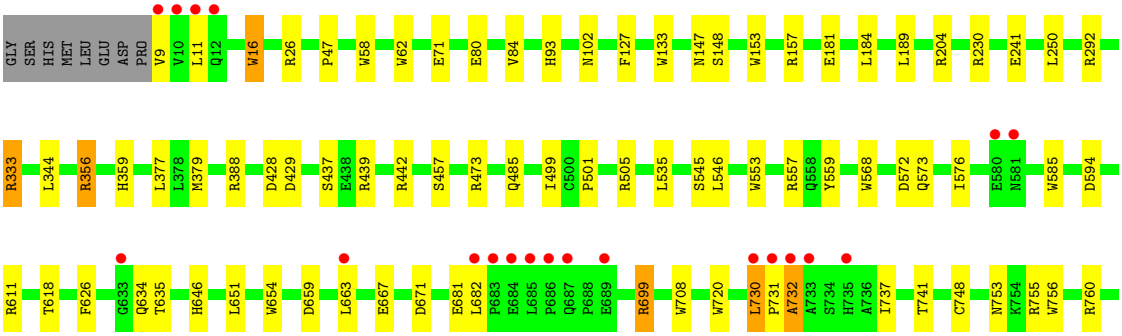
• Molecule 1: Beta-galactosidase

Chain A:



• Molecule 1: Beta-galactosidase

Chain B:



M768 W769 T778 T799 R800 W806 R809 W810 A820 W842 R853 N885 W897 Q903 R909 R917 W918 Y962 L976 W983 L1018 V1019 W1020 C1021 Q1022 K1023

• Molecule 1: Beta-galactosidase

Chain C: 2% 88% 10%

GLY SER HIS MET LEU GLU ASP PRO V9 V10 L11 Q12 W16 R26 F33 P47 S48 Q49 L54 W62 E71 S72 W73 E80 S88 N102 F127 Q135 N147 S148 W153 W158 G162 E181 L184 L189 R190 W191 W203

D211 L214 D224 R230 E241 M246 L250 R251 D252 R255 Q262 D287 R288 V289 R292 P306 R333 L344 R356 V366 M367 M372 M379 L397 W398 T427 R431 W432 L433 E438 R439 R442 S462 R473 W474

D492 D509 K521 K522 W523 P527 L535 L546 W553 Y559 E580 W585 T618 F626 R630 G633 Q634 H646 L651 L652 H653 W654 M655 P662 S665 G666 D671 E681 L682 P683 E684 L685 P686 Q687 P688 E689 R699 W720

L730 P731 A732 A733 S734 H735 A736 I737 P738 H739 M745 I770 G771 D772 K773 T778 A798 T799 R800 L830 W842 R853 K854 T855 Q890 V891 Q903 R909 L910 R917 W918 R938 R961 Q965 E969 L984 R1013 W1020 K1023

• Molecule 1: Beta-galactosidase

Chain D: 3% 89% 9%

GLY SER HIS MET LEU GLU ASP PRO V9 V10 L11 Q12 R13 R14 D15 W16 R37 W62 E67 E71 S72 W73 P79 E80 S88 N102 P112 Q135 E136 S174 R204 D233 D234 R237 E241 M246 L250 R251 D252 R292 E296

W301 E324 R333 L344 R356 V366 L377 W398 Y399 T400 D403 R425 D428 R431 W432 L433 P434 R439 R442 R446 R473 W474 S477 D492 I499 C500 P501 K521 F549 W553 R557 Q558 Y559 D572 E580 N581

W585 T595 P596 P615 T618 E619 A620 Q634 H653 L663 D671 L682 P683 E684 L685 P686 Q687 P688 E689 W695 R699 V700 V701 W708 I714 T729 L730 P731 A732 A733 S734 H735 A736 I737 P738 M745 R755 W756 M768 D772 Q775

T778 A798 T799 R800 N804 R809 W810 L830 Q845 R881 Q887 Q890 V891 A892 W897 P907 D908 R909 A912 E980 R1013 Q1022 K1023

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.29Å 168.10Å 200.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.81 – 1.60 53.76 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (55.81-1.60) 92.1 (53.76-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.188 0.159 , 0.187	Depositor DCC
R_{free} test set	8778 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	38364	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 35.68 % 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 5.6165e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DMS, CL, K, MG, CSD

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	1.08	18/8684 (0.2%)	1.09	36/11840 (0.3%)
1	B	1.07	17/8628 (0.2%)	1.07	28/11769 (0.2%)
1	C	1.06	17/8651 (0.2%)	1.06	33/11798 (0.3%)
1	D	1.07	14/8652 (0.2%)	1.06	29/11804 (0.2%)
All	All	1.07	66/34615 (0.2%)	1.07	126/47211 (0.3%)

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	B	0	1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	810	TRP	CD2-CE2	7.17	1.50	1.41
1	B	897	TRP	CD2-CE2	6.76	1.49	1.41
1	C	585	TRP	CD2-CE2	6.69	1.49	1.41
1	B	918	TRP	CD2-CE2	6.58	1.49	1.41
1	A	203	TRP	CD2-CE2	6.52	1.49	1.41

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	442	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	C	442	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	C	431[A]	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	C	431[B]	ARG	NE-CZ-NH2	-9.85	115.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	ARG	NE-CZ-NH1	9.70	125.15	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1022	GLN	Peptide

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	8365	0	8028	68	0
1	B	8315	0	7967	67	0
1	C	8342	0	7991	68	0
1	D	8328	0	8000	52	0
2	A	4	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
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	1	0	0	0	0
5	A	128	0	192	27	0
5	B	148	0	222	27	0
5	C	148	0	222	26	0
5	D	108	0	162	12	0
6	A	1130	0	0	15	1
6	B	1114	0	0	13	1
6	C	1094	0	0	26	2
6	D	1113	0	0	17	2
All	All	38364	0	32784	278	3

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 4.

The worst 5 of 278 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:B:576:ILE:CD1	5:B:1119:DMS:C2	2.07	1.33
1:B:576:ILE:HD12	5:B:1119:DMS:C2	1.65	1.26
1:A:430:PRO:HD3	5:A:3025:DMS:C1	1.69	1.23
1:B:576:ILE:CD1	5:B:1119:DMS:H22	1.77	1.12
1:A:651[B]:LEU:HD21	1:A:667:GLU:HB3	1.33	1.07

All (3) 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)
6:B:1256:HOH:O	6:C:3103:HOH:O[4_455]	1.79	0.41
6:A:3193:HOH:O	6:D:1263:HOH:O[4_545]	2.03	0.17
6:C:3129:HOH:O	6:D:1243:HOH:O[2_554]	2.11	0.09

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	1047/1023 (102%)	1019 (97%)	28 (3%)	0	100	100
1	B	1041/1023 (102%)	1011 (97%)	29 (3%)	1 (0%)	51	29
1	C	1043/1023 (102%)	1014 (97%)	29 (3%)	0	100	100
1	D	1045/1023 (102%)	1022 (98%)	23 (2%)	0	100	100
All	All	4176/4092 (102%)	4066 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA

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	902/874 (103%)	883 (98%)	19 (2%)	53	29
1	B	896/874 (102%)	883 (98%)	13 (2%)	65	44
1	C	898/874 (103%)	878 (98%)	20 (2%)	52	27
1	D	900/874 (103%)	888 (99%)	12 (1%)	69	50
All	All	3596/3496 (103%)	3532 (98%)	64 (2%)	59	36

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	663	LEU
1	D	735	HIS
1	B	535	LEU
1	B	344	LEU
1	D	737	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	739	HIS
1	D	102	ASN
1	B	775	GLN
1	C	102	ASN
1	C	135	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)

4 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	CSD	B	247	1	3,7,8	1.02	0	1,8,10	0.63	0
1	CSD	C	247	1	3,7,8	1.26	0	1,8,10	0.89	0
1	CSD	A	247	1	3,7,8	0.90	0	1,8,10	2.88	1 (100%)
1	CSD	D	247	1	3,7,8	1.06	0	1,8,10	1.89	0

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	CSD	B	247	1	-	1/2/6/8	-
1	CSD	C	247	1	-	1/2/6/8	-
1	CSD	A	247	1	-	2/2/6/8	-
1	CSD	D	247	1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	CSD	OD1-SG-CB	-2.88	100.06	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	247	CSD	CA-CB-SG-OD1
1	B	247	CSD	CA-CB-SG-OD1
1	C	247	CSD	CA-CB-SG-OD1
1	D	247	CSD	CA-CB-SG-OD1
1	A	247	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
5	DMS	B	1115	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	D	1129	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	C	3033	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1113	-	3,3,3	0.54	0	3,3,3	0.46	0
5	DMS	A	3014	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	D	1131	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3041	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3036	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1132	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	C	3019	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3020	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1111	-	3,3,3	0.53	0	3,3,3	0.49	0
5	DMS	C	3040	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3023	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3012	-	3,3,3	0.53	0	3,3,3	0.48	0
5	DMS	D	1119	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	D	1133	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3009	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	A	3011	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3013	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	A	3039	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1121	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1122	-	3,3,3	0.54	0	3,3,3	0.54	0
5	DMS	B	1139	-	3,3,3	0.54	0	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	C	3011	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	C	3022	-	3,3,3	0.53	0	3,3,3	0.49	0
5	DMS	C	3045	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	D	1125	-	3,3,3	0.53	0	3,3,3	0.49	0
5	DMS	A	3032	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	A	3040	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	B	1129	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3032	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1137	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1124	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3029	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	D	1112[A]	-	3,3,3	0.55	0	3,3,3	0.52	0
5	DMS	C	3038	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1101	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3021	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3035	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1101	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3034	-	3,3,3	0.55	0	3,3,3	0.48	0
5	DMS	B	1120	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3038	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3020	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	C	3042	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3018	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3037	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3026	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3030	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	D	1113	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	C	3027	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3024	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	D	1123	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3022	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3043	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	B	1123	-	3,3,3	0.53	0	3,3,3	0.51	0
5	DMS	D	1132	-	3,3,3	0.55	0	3,3,3	0.49	0
5	DMS	B	1135	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1126	-	3,3,3	0.55	0	3,3,3	0.50	0
5	DMS	A	3025	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3021	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	B	1133	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1114	-	3,3,3	0.53	0	3,3,3	0.48	0
5	DMS	C	3025	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1119	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3010	-	3,3,3	0.53	0	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	B	1121	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3010	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	D	1117	-	3,3,3	0.55	0	3,3,3	0.50	0
5	DMS	C	3031	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1117	-	3,3,3	0.54	0	3,3,3	0.52	0
5	DMS	B	1118	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1144	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1109	-	3,3,3	0.54	0	3,3,3	0.46	0
5	DMS	B	1140	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1127	-	3,3,3	0.53	0	3,3,3	0.42	0
5	DMS	C	3030	-	3,3,3	0.53	0	3,3,3	0.49	0
5	DMS	B	1143	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3017	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3027	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3023	-	3,3,3	0.55	0	3,3,3	0.53	0
5	DMS	A	3012	-	3,3,3	0.53	0	3,3,3	0.48	0
5	DMS	B	1102	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1130	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1128	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3028	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3018	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3029	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	B	1130	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1141	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3013	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	B	1136	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3044	-	3,3,3	0.55	0	3,3,3	0.50	0
5	DMS	D	1115	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1124	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1112	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1103	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	B	1116	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3035	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3016	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3031	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	D	1114	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	B	1134	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	B	1138	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	D	1126	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1127	-	3,3,3	0.55	0	3,3,3	0.51	0
5	DMS	A	3026	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3017	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	C	3014	-	3,3,3	0.55	0	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	D	1116	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	B	1125	-	3,3,3	0.54	0	3,3,3	0.52	0
5	DMS	D	1128	-	3,3,3	0.53	0	3,3,3	0.49	0
5	DMS	B	1142	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1110	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	B	1131	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	A	3028	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1111	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	A	3041	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3024	-	3,3,3	0.55	0	3,3,3	0.51	0
5	DMS	C	3037	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3015	-	3,3,3	0.55	0	3,3,3	0.50	0
5	DMS	A	3036	-	3,3,3	0.54	0	3,3,3	0.51	0
5	DMS	A	3016	-	3,3,3	0.54	0	3,3,3	0.48	0
5	DMS	D	1112[B]	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	C	3015	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1118	-	3,3,3	0.55	0	3,3,3	0.51	0
5	DMS	A	3034	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1120	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	D	1122	-	3,3,3	0.54	0	3,3,3	0.49	0
5	DMS	C	3039	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3019	-	3,3,3	0.54	0	3,3,3	0.50	0
5	DMS	A	3033	-	3,3,3	0.54	0	3,3,3	0.50	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.

29 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1129	DMS	4	0
5	C	3036	DMS	2	0
5	B	1132	DMS	2	0
5	C	3019	DMS	4	0
5	C	3023	DMS	2	0
5	B	1122	DMS	7	0
5	C	3032	DMS	2	0
5	D	1101	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3034	DMS	7	0
5	A	3038	DMS	1	0
5	A	3025	DMS	10	0
5	B	1119	DMS	10	0
5	C	3030	DMS	1	0
5	A	3027	DMS	3	0
5	A	3023	DMS	4	0
5	C	3029	DMS	4	0
5	B	1130	DMS	1	0
5	C	3044	DMS	1	0
5	A	3031	DMS	1	0
5	D	1126	DMS	1	0
5	B	1127	DMS	4	0
5	A	3026	DMS	2	0
5	B	1125	DMS	3	0
5	A	3028	DMS	1	0
5	A	3041	DMS	2	0
5	A	3024	DMS	3	0
5	C	3015	DMS	2	0
5	D	1122	DMS	5	0
5	C	3039	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 (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	1014/1023 (99%)	-0.30	30 (2%)	50	48	6, 12, 30, 90	0
1	B	1014/1023 (99%)	-0.36	22 (2%)	62	60	6, 12, 28, 74	0
1	C	1014/1023 (99%)	-0.30	24 (2%)	59	56	7, 12, 32, 79	0
1	D	1014/1023 (99%)	-0.25	31 (3%)	49	46	6, 13, 31, 79	0
All	All	4056/4092 (99%)	-0.30	107 (2%)	56	53	6, 12, 30, 90	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	10.8
1	D	732	ALA	8.6
1	D	735	HIS	7.3
1	A	735	HIS	6.3
1	D	689	GLU	6.3

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	CSD	A	247	8/9	0.95	0.10	9,11,21,22	0
1	CSD	C	247	8/9	0.96	0.07	11,14,24,25	0
1	CSD	B	247	8/9	0.97	0.09	11,13,25,27	0
1	CSD	D	247	8/9	0.97	0.07	10,12,21,23	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(Å^2)	Q<0.9
5	DMS	C	3036	4/4	0.72	0.18	24,27,29,34	4
5	DMS	B	1140	4/4	0.80	0.19	19,20,24,27	4
5	DMS	A	3037	4/4	0.83	0.16	31,41,41,50	4
5	DMS	B	1137	4/4	0.83	0.16	32,34,35,44	4
5	DMS	B	1142	4/4	0.85	0.17	22,24,31,33	4
5	DMS	A	3015	4/4	0.85	0.15	23,29,36,47	4
5	DMS	C	3043	4/4	0.85	0.20	43,46,49,50	4
2	MG	B	1106	1/1	0.86	0.10	25,25,25,25	1
5	DMS	B	1103	4/4	0.86	0.17	42,45,48,53	4
5	DMS	B	1125	4/4	0.86	0.13	29,29,36,36	4
5	DMS	A	3030	4/4	0.86	0.18	19,21,30,30	4
5	DMS	C	3035	4/4	0.87	0.15	45,48,51,59	0
5	DMS	B	1136	4/4	0.87	0.13	35,48,50,51	0
5	DMS	C	3038	4/4	0.87	0.14	26,31,32,35	4
5	DMS	C	3030	4/4	0.87	0.16	27,29,33,36	4
5	DMS	B	1138	4/4	0.88	0.16	32,34,38,39	4
2	MG	A	3003	1/1	0.88	0.12	28,28,28,28	1
5	DMS	B	1130	4/4	0.88	0.19	22,25,26,29	4
5	DMS	C	3024	4/4	0.88	0.14	25,27,37,38	4
5	DMS	C	3029	4/4	0.88	0.18	19,21,26,32	4
5	DMS	B	1143	4/4	0.90	0.15	40,41,51,52	4
5	DMS	C	3015	4/4	0.90	0.17	18,22,23,24	4
5	DMS	A	3035	4/4	0.90	0.15	46,48,49,53	4
5	DMS	C	3032	4/4	0.91	0.14	25,27,29,34	4
5	DMS	A	3024	4/4	0.91	0.16	16,26,26,35	4
5	DMS	A	3040	4/4	0.91	0.15	21,22,30,31	4
5	DMS	A	3027	4/4	0.91	0.16	22,28,30,32	4
5	DMS	C	3041	4/4	0.91	0.14	18,21,28,31	4
5	DMS	C	3042	4/4	0.91	0.14	35,36,37,40	4
5	DMS	B	1121	4/4	0.91	0.16	23,24,26,26	4
5	DMS	D	1129	4/4	0.91	0.17	23,26,27,33	4
5	DMS	D	1130	4/4	0.91	0.13	45,47,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	1131	4/4	0.92	0.13	21,26,30,30	0
5	DMS	A	3025	4/4	0.92	0.19	22,24,29,31	4
5	DMS	C	3037	4/4	0.92	0.14	27,30,31,36	4
5	DMS	C	3022	4/4	0.92	0.13	18,20,23,24	4
5	DMS	C	3040	4/4	0.92	0.17	43,46,48,48	4
5	DMS	B	1126	4/4	0.92	0.17	29,39,44,54	0
5	DMS	C	3025	4/4	0.92	0.17	20,21,22,23	4
5	DMS	B	1128	4/4	0.92	0.13	29,33,34,36	4
5	DMS	D	1115	4/4	0.92	0.18	15,15,16,20	4
5	DMS	B	1129	4/4	0.92	0.13	18,20,23,25	4
5	DMS	A	3041	4/4	0.92	0.18	34,34,36,40	4
5	DMS	C	3028	4/4	0.93	0.13	41,42,44,49	4
5	DMS	D	1123	4/4	0.93	0.18	37,39,44,50	4
5	DMS	D	1126	4/4	0.93	0.12	22,26,26,30	4
5	DMS	D	1128	4/4	0.93	0.13	18,19,19,20	4
5	DMS	A	3023	4/4	0.93	0.20	23,31,32,40	0
5	DMS	C	3023	4/4	0.93	0.25	37,37,41,45	4
5	DMS	D	1131	4/4	0.93	0.08	45,48,50,59	0
5	DMS	B	1116	4/4	0.94	0.12	15,18,18,18	4
5	DMS	A	3022	4/4	0.94	0.17	22,22,23,24	4
5	DMS	A	3036	4/4	0.94	0.10	34,35,42,44	4
5	DMS	A	3016	4/4	0.94	0.16	14,14,16,18	4
5	DMS	B	1139	4/4	0.94	0.11	35,37,43,43	4
5	DMS	C	3045	4/4	0.94	0.13	33,34,36,38	4
5	DMS	D	1112[A]	4/4	0.94	0.11	16,16,19,21	4
5	DMS	D	1112[B]	4/4	0.94	0.11	14,15,15,17	4
5	DMS	B	1127	4/4	0.94	0.18	19,24,29,30	4
5	DMS	D	1121	4/4	0.94	0.14	20,23,24,25	4
5	DMS	D	1122	4/4	0.94	0.16	21,30,33,35	4
5	DMS	A	3028	4/4	0.94	0.13	40,44,47,49	4
5	DMS	D	1125	4/4	0.94	0.12	17,20,23,23	4
5	DMS	C	3031	4/4	0.94	0.12	36,36,40,47	0
5	DMS	A	3029	4/4	0.94	0.11	14,16,18,18	4
5	DMS	B	1144	4/4	0.94	0.12	37,39,41,46	4
5	DMS	A	3018	4/4	0.94	0.10	23,23,25,28	4
5	DMS	C	3020	4/4	0.94	0.16	23,24,27,27	4
5	DMS	B	1114	4/4	0.95	0.12	13,14,17,18	4
3	K	D	1108	1/1	0.95	0.09	16,16,16,16	1
5	DMS	C	3027	4/4	0.95	0.12	22,28,30,31	4
5	DMS	D	1101	4/4	0.95	0.11	25,26,26,29	4
5	DMS	A	3031	4/4	0.95	0.11	22,23,25,26	4
5	DMS	B	1123	4/4	0.95	0.10	16,19,22,23	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	1133	4/4	0.95	0.10	20,21,25,25	4
5	DMS	C	3012	4/4	0.95	0.11	14,15,16,17	0
5	DMS	C	3014	4/4	0.95	0.12	16,19,21,21	4
5	DMS	B	1134	4/4	0.95	0.10	23,23,25,25	4
5	DMS	D	1124	4/4	0.95	0.10	40,46,48,55	4
5	DMS	C	3016	4/4	0.95	0.09	23,23,24,24	4
5	DMS	C	3017	4/4	0.95	0.13	19,22,23,24	4
5	DMS	D	1127	4/4	0.95	0.11	9,10,11,16	4
5	DMS	A	3021	4/4	0.95	0.14	23,26,27,27	4
5	DMS	C	3039	4/4	0.95	0.15	35,35,40,46	4
5	DMS	B	1101	4/4	0.95	0.10	45,46,47,54	0
5	DMS	A	3017	4/4	0.95	0.09	22,25,29,30	0
5	DMS	D	1133	4/4	0.95	0.11	23,26,28,28	4
5	DMS	C	3021	4/4	0.96	0.14	19,33,33,36	0
5	DMS	B	1118	4/4	0.96	0.09	20,21,22,24	0
5	DMS	B	1119	4/4	0.96	0.11	13,16,19,22	4
5	DMS	A	3032	4/4	0.96	0.13	19,24,25,30	4
5	DMS	B	1102	4/4	0.96	0.16	41,43,44,46	4
5	DMS	B	1124	4/4	0.96	0.13	23,27,28,28	4
5	DMS	C	3013	4/4	0.96	0.09	20,21,21,23	0
5	DMS	B	1135	4/4	0.96	0.11	34,39,42,47	0
5	DMS	C	3044	4/4	0.96	0.13	20,20,22,23	4
5	DMS	A	3038	4/4	0.96	0.10	20,20,22,28	4
5	DMS	A	3026	4/4	0.96	0.15	33,33,36,38	4
5	DMS	A	3013	4/4	0.96	0.10	12,13,14,15	4
5	DMS	B	1117	4/4	0.96	0.09	21,24,25,28	4
5	DMS	D	1117	4/4	0.97	0.09	21,21,22,22	4
5	DMS	B	1141	4/4	0.97	0.13	34,34,38,42	4
5	DMS	A	3012	4/4	0.97	0.08	16,16,17,18	4
5	DMS	C	3019	4/4	0.97	0.14	21,26,29,34	0
5	DMS	B	1122	4/4	0.97	0.15	20,29,31,32	4
3	K	C	3008	1/1	0.97	0.07	16,16,16,16	1
5	DMS	A	3019	4/4	0.97	0.11	19,21,21,22	4
5	DMS	C	3034	4/4	0.97	0.11	22,22,23,23	4
5	DMS	A	3033	4/4	0.97	0.11	33,46,49,51	0
5	DMS	B	1132	4/4	0.97	0.12	19,19,21,22	4
5	DMS	A	3039	4/4	0.97	0.15	23,33,33,34	4
5	DMS	C	3026	4/4	0.97	0.07	27,27,29,31	4
5	DMS	D	1132	4/4	0.97	0.14	20,30,31,35	4
5	DMS	D	1116	4/4	0.97	0.09	22,24,25,33	0
5	DMS	A	3011	4/4	0.98	0.09	12,12,12,12	4
3	K	B	1110	1/1	0.98	0.07	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	D	1118	4/4	0.98	0.10	19,20,22,23	4
5	DMS	D	1119	4/4	0.98	0.07	17,21,21,23	4
2	MG	A	3004	1/1	0.98	0.07	14,14,14,14	1
5	DMS	B	1112	4/4	0.98	0.08	14,14,14,15	0
5	DMS	A	3014	4/4	0.98	0.08	19,19,21,21	0
5	DMS	B	1115	4/4	0.98	0.07	18,18,21,22	4
5	DMS	A	3020	4/4	0.98	0.08	16,18,20,24	4
5	DMS	C	3033	4/4	0.98	0.09	32,38,39,40	0
5	DMS	C	3010	4/4	0.98	0.08	16,16,16,16	0
5	DMS	D	1111	4/4	0.98	0.06	15,15,17,17	4
5	DMS	C	3011	4/4	0.98	0.06	17,17,17,19	0
2	MG	C	3003	1/1	0.98	0.16	17,17,17,17	1
5	DMS	D	1113	4/4	0.98	0.08	17,18,20,21	0
5	DMS	D	1114	4/4	0.98	0.08	14,15,16,17	0
5	DMS	A	3034	4/4	0.98	0.10	43,43,43,44	4
5	DMS	A	3010	4/4	0.99	0.06	10,11,11,12	0
5	DMS	C	3009	4/4	0.99	0.06	11,12,13,13	0
2	MG	D	1103	1/1	0.99	0.06	13,13,13,13	0
5	DMS	B	1120	4/4	0.99	0.08	19,23,23,23	4
5	DMS	D	1120	4/4	0.99	0.08	18,20,21,23	4
2	MG	D	1104	1/1	0.99	0.04	14,14,14,14	1
3	K	A	3007	1/1	0.99	0.04	12,12,12,12	0
3	K	A	3008	1/1	0.99	0.07	14,14,14,14	1
5	DMS	B	1111	4/4	0.99	0.06	10,12,13,13	0
2	MG	A	3002	1/1	0.99	0.09	10,10,10,10	1
5	DMS	D	1109	4/4	0.99	0.05	9,10,11,12	0
5	DMS	D	1110	4/4	0.99	0.06	12,12,12,14	0
5	DMS	B	1113	4/4	0.99	0.05	16,17,17,18	0
5	DMS	C	3018	4/4	0.99	0.07	16,19,20,23	4
2	MG	C	3004	1/1	0.99	0.06	9,9,9,9	1
3	K	D	1107	1/1	0.99	0.04	12,12,12,12	0
2	MG	D	1102	1/1	0.99	0.05	8,8,8,8	1
4	CL	A	3009	1/1	0.99	0.05	19,19,19,19	0
3	K	A	3005	1/1	1.00	0.03	18,18,18,18	0
3	K	A	3006	1/1	1.00	0.10	5,5,5,5	1
2	MG	B	1104	1/1	1.00	0.05	7,7,7,7	1
2	MG	B	1105	1/1	1.00	0.07	12,12,12,12	0
3	K	B	1107	1/1	1.00	0.03	15,15,15,15	0
3	K	B	1108	1/1	1.00	0.05	7,7,7,7	0
3	K	B	1109	1/1	1.00	0.05	11,11,11,11	0
2	MG	A	3001	1/1	1.00	0.04	8,8,8,8	1
3	K	C	3005	1/1	1.00	0.03	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	C	3006	1/1	1.00	0.06	8,8,8,8	0
3	K	C	3007	1/1	1.00	0.05	11,11,11,11	0
2	MG	C	3001	1/1	1.00	0.04	8,8,8,8	1
3	K	D	1105	1/1	1.00	0.05	18,18,18,18	0
3	K	D	1106	1/1	1.00	0.06	7,7,7,7	0
2	MG	C	3002	1/1	1.00	0.07	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.