Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 04:47 AM EDT

PDB ID	:	4DUV
Title	:	E. coli (lacZ) beta-galactosidase (G974A) 2-deoxy-galactosyl-enzyme and bis-Tris complex
Authors	:	Wheatley, R.W.; Lo, S.; Janzcewicz, L.J.; Dugdale, M.L.; Huber, R.E.
Deposited on	:	2012-02-22
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*
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:

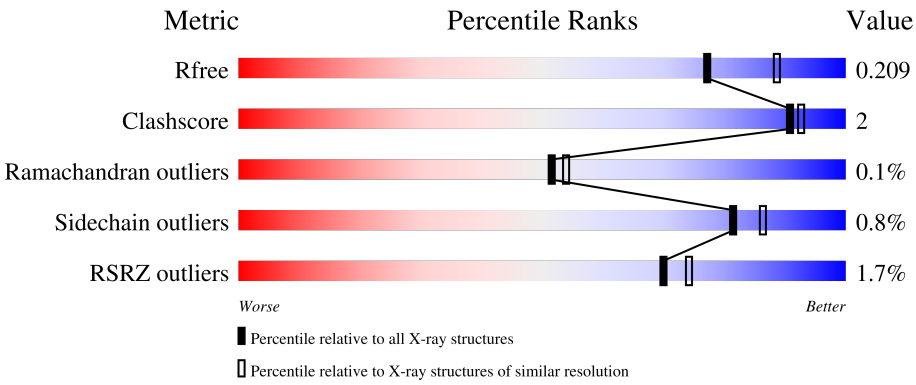
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 >=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	1052	2% 93%
1	B	1052	% 92% 5%
1	C	1052	2% 93%
1	D	1052	2% 92% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 37231 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	1019	8189	5180	1449	1521	39	0	0	0
1	B	1018	8181	5175	1448	1520	38	0	0	0
1	C	1018	8181	5175	1448	1520	38	0	0	0
1	D	1018	8181	5175	1448	1520	38	0	0	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP P00722
A	-27	GLY	-	expression tag	UNP P00722
A	-26	GLY	-	expression tag	UNP P00722
A	-25	SER	-	expression tag	UNP P00722
A	-24	HIS	-	expression tag	UNP P00722
A	-23	HIS	-	expression tag	UNP P00722
A	-22	HIS	-	expression tag	UNP P00722
A	-21	HIS	-	expression tag	UNP P00722
A	-20	HIS	-	expression tag	UNP P00722
A	-19	HIS	-	expression tag	UNP P00722
A	-18	GLY	-	expression tag	UNP P00722
A	-17	MET	-	expression tag	UNP P00722
A	-16	ALA	-	expression tag	UNP P00722
A	-15	SER	-	expression tag	UNP P00722
A	-14	MET	-	expression tag	UNP P00722
A	-13	THR	-	expression tag	UNP P00722
A	-12	GLY	-	expression tag	UNP P00722
A	-11	GLY	-	expression tag	UNP P00722
A	-10	GLN	-	expression tag	UNP P00722
A	-9	GLN	-	expression tag	UNP P00722
A	-8	MET	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P00722
A	-6	ARG	-	expression tag	UNP P00722
A	-5	ASP	-	expression tag	UNP P00722
A	-4	LEU	-	expression tag	UNP P00722
A	-3	TYR	-	expression tag	UNP P00722
A	-2	ASP	-	expression tag	UNP P00722
A	-1	ASP	-	expression tag	UNP P00722
A	0	ASP	-	expression tag	UNP P00722
A	1	ASP	-	expression tag	UNP P00722
A	2	LYS	-	expression tag	UNP P00722
A	3	ASP	-	expression tag	UNP P00722
A	4	PRO	-	expression tag	UNP P00722
A	5	MET	-	expression tag	UNP P00722
A	6	ILE	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	794	ALA	GLY	engineered mutation	UNP P00722
B	-28	MET	-	initiating methionine	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	TYR	-	expression tag	UNP P00722
B	-2	ASP	-	expression tag	UNP P00722
B	-1	ASP	-	expression tag	UNP P00722
B	0	ASP	-	expression tag	UNP P00722
B	1	ASP	-	expression tag	UNP P00722
B	2	LYS	-	expression tag	UNP P00722
B	3	ASP	-	expression tag	UNP P00722
B	4	PRO	-	expression tag	UNP P00722
B	5	MET	-	expression tag	UNP P00722
B	6	ILE	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	794	ALA	GLY	engineered mutation	UNP P00722
C	-28	MET	-	initiating methionine	UNP P00722
C	-27	GLY	-	expression tag	UNP P00722
C	-26	GLY	-	expression tag	UNP P00722
C	-25	SER	-	expression tag	UNP P00722
C	-24	HIS	-	expression tag	UNP P00722
C	-23	HIS	-	expression tag	UNP P00722
C	-22	HIS	-	expression tag	UNP P00722
C	-21	HIS	-	expression tag	UNP P00722
C	-20	HIS	-	expression tag	UNP P00722
C	-19	HIS	-	expression tag	UNP P00722
C	-18	GLY	-	expression tag	UNP P00722
C	-17	MET	-	expression tag	UNP P00722
C	-16	ALA	-	expression tag	UNP P00722
C	-15	SER	-	expression tag	UNP P00722
C	-14	MET	-	expression tag	UNP P00722
C	-13	THR	-	expression tag	UNP P00722
C	-12	GLY	-	expression tag	UNP P00722
C	-11	GLY	-	expression tag	UNP P00722
C	-10	GLN	-	expression tag	UNP P00722
C	-9	GLN	-	expression tag	UNP P00722
C	-8	MET	-	expression tag	UNP P00722
C	-7	GLY	-	expression tag	UNP P00722
C	-6	ARG	-	expression tag	UNP P00722
C	-5	ASP	-	expression tag	UNP P00722
C	-4	LEU	-	expression tag	UNP P00722
C	-3	TYR	-	expression tag	UNP P00722
C	-2	ASP	-	expression tag	UNP P00722
C	-1	ASP	-	expression tag	UNP P00722
C	0	ASP	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	794	ALA	GLY	engineered mutation	UNP P00722
D	-28	MET	-	expression tag	UNP P00722
D	-27	GLY	-	expression tag	UNP P00722
D	-26	GLY	-	expression tag	UNP P00722
D	-25	SER	-	expression tag	UNP P00722
D	-24	HIS	-	expression tag	UNP P00722
D	-23	HIS	-	expression tag	UNP P00722
D	-22	HIS	-	expression tag	UNP P00722
D	-21	HIS	-	expression tag	UNP P00722
D	-20	HIS	-	expression tag	UNP P00722
D	-19	HIS	-	expression tag	UNP P00722
D	-18	GLY	-	expression tag	UNP P00722
D	-17	MET	-	expression tag	UNP P00722
D	-16	ALA	-	expression tag	UNP P00722
D	-15	SER	-	expression tag	UNP P00722
D	-14	MET	-	expression tag	UNP P00722
D	-13	THR	-	expression tag	UNP P00722
D	-12	GLY	-	expression tag	UNP P00722
D	-11	GLY	-	expression tag	UNP P00722
D	-10	GLN	-	expression tag	UNP P00722
D	-9	GLN	-	expression tag	UNP P00722
D	-8	MET	-	expression tag	UNP P00722
D	-7	GLY	-	expression tag	UNP P00722
D	-6	ARG	-	expression tag	UNP P00722
D	-5	ASP	-	expression tag	UNP P00722
D	-4	LEU	-	expression tag	UNP P00722
D	-3	TYR	-	expression tag	UNP P00722
D	-2	ASP	-	expression tag	UNP P00722
D	-1	ASP	-	expression tag	UNP P00722
D	0	ASP	-	expression tag	UNP P00722
D	1	ASP	-	expression tag	UNP P00722
D	2	LYS	-	expression tag	UNP P00722
D	3	ASP	-	expression tag	UNP P00722
D	4	PRO	-	expression tag	UNP P00722

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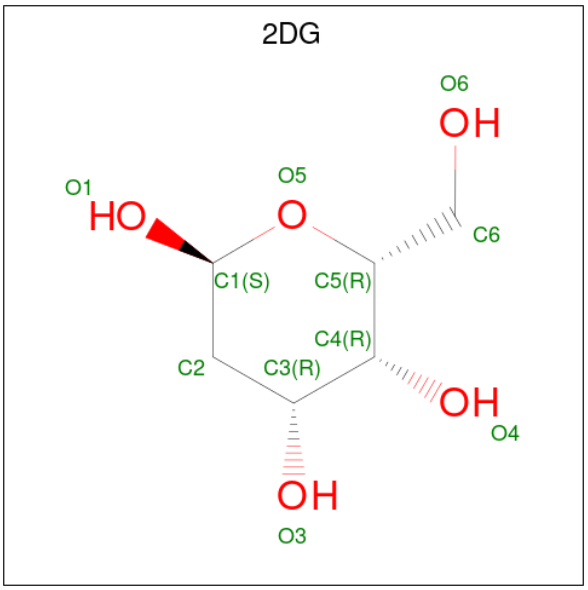
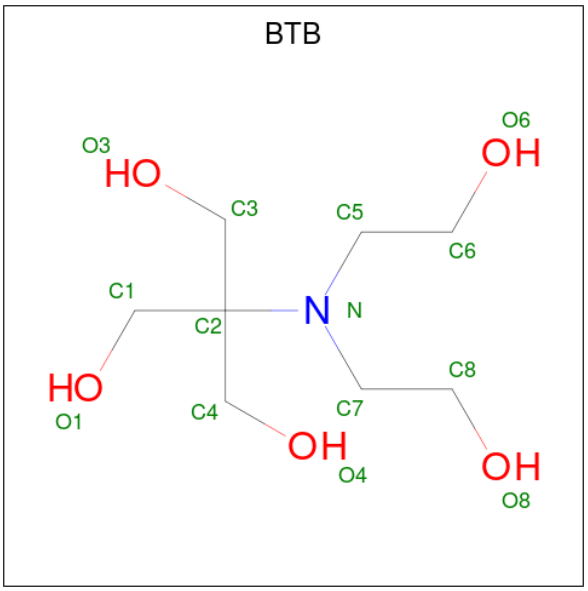
Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	794	ALA	GLY	engineered mutation	UNP P00722

- Molecule 2 is 2-deoxy-alpha-D-galactopyranose (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			10	6	4			
2	B	1	Total	C	O		0	0
			10	6	4			
2	C	1	Total	C	O		0	0
			10	6	4			
2	D	1	Total	C	O		0	0
			10	6	4			

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Na 4 4	0	0

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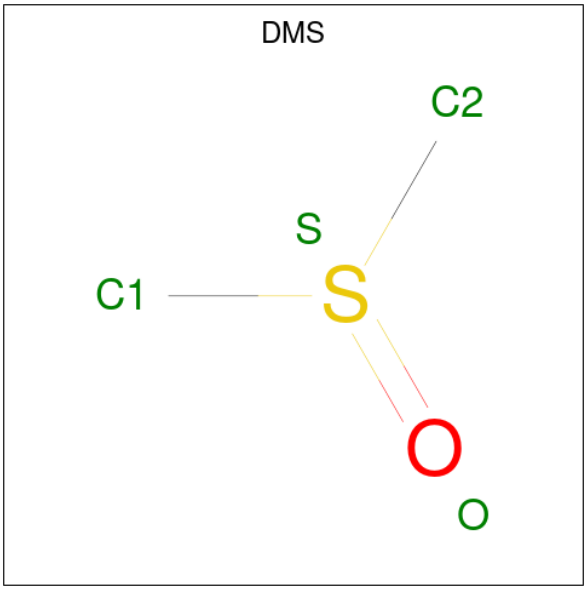
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total Na 4 4	0	0
5	C	4	Total Na 4 4	0	0
5	D	4	Total Na 4 4	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

- Molecule 7 is water.

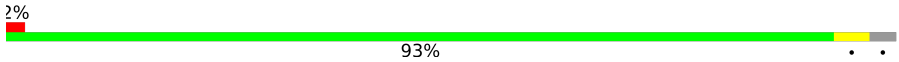
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	1039	1039	1039	0	0
			Total	O		
7	B	973	973	973	0	0
			Total	O		
7	C	994	994	994	0	0
			Total	O		
7	D	1012	1012	1012	0	0

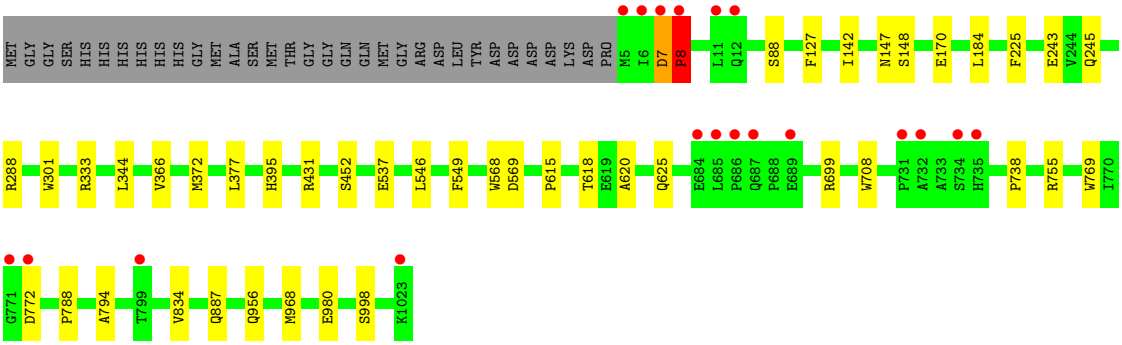
3 Residue-property plots (i)

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

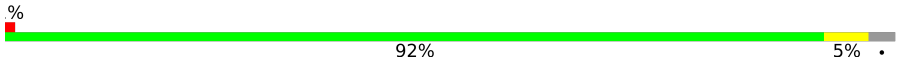
Chain A:

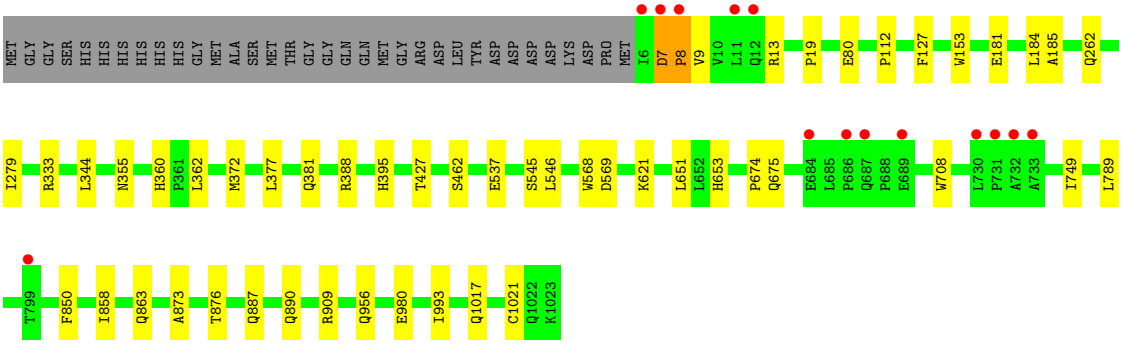




• Molecule 1: Beta-galactosidase

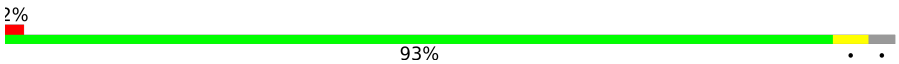
Chain B:

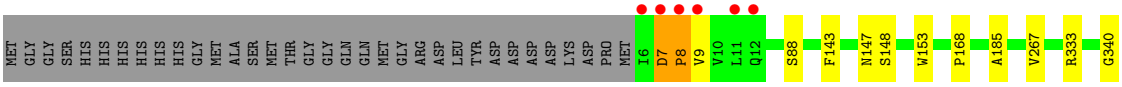


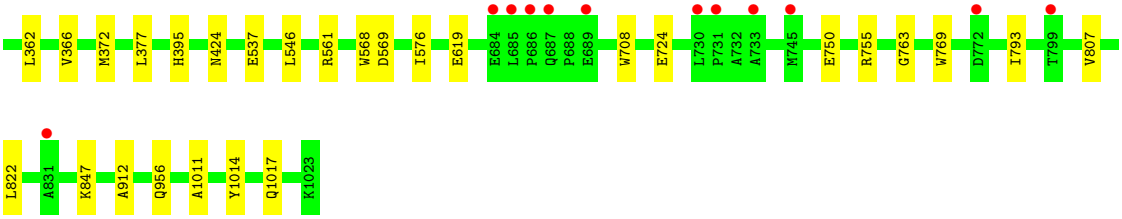


• Molecule 1: Beta-galactosidase

Chain C:

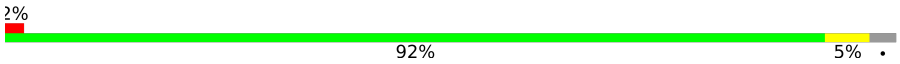


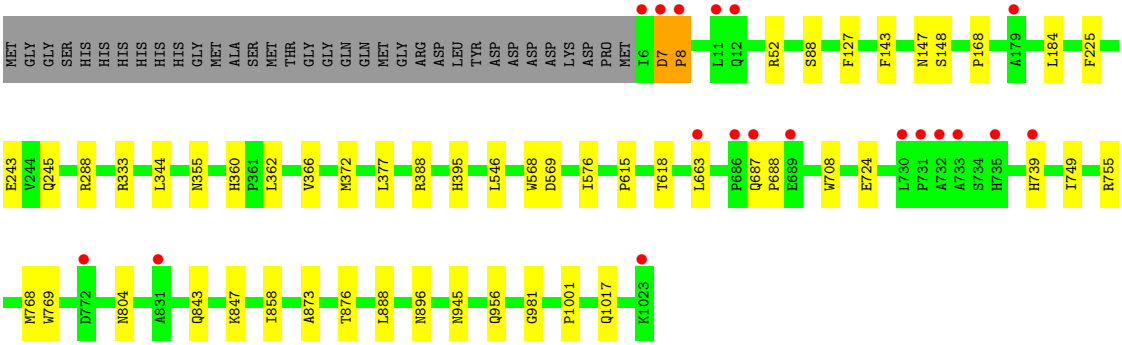




• Molecule 1: Beta-galactosidase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	150.57Å 167.73Å 201.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.41 – 2.10 86.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.41-2.10) 100.0 (86.41-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.158 , 0.206 0.162 , 0.209	Depositor DCC
R_{free} test set	4267 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	37231	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 38.76 % 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 3.5103e-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: BTB, 2DG, 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	0.39	0/8432	0.54	0/11504
1	B	0.39	0/8424	0.53	0/11494
1	C	0.38	0/8424	0.52	0/11494
1	D	0.38	0/8424	0.53	0/11494
All	All	0.38	0/33704	0.53	0/45986

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	8189	0	7786	23	0
1	B	8181	0	7777	29	0
1	C	8181	0	7777	23	0
1	D	8181	0	7777	28	0
2	A	10	0	9	1	0
2	B	10	0	9	1	0
2	C	10	0	9	1	0
2	D	10	0	9	0	0
3	A	14	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	19	2	0
3	C	14	0	19	2	0
3	D	14	0	19	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	76	0	114	0	0
6	B	96	0	144	0	0
6	C	100	0	150	1	0
6	D	88	0	132	0	0
7	A	1039	0	0	5	0
7	B	973	0	0	3	0
7	C	994	0	0	0	0
7	D	1012	0	0	4	0
All	All	37231	0	31769	108	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 2.

All (108) 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)
3:A:2101:BTB:H31	7:A:5025:HOH:O	1.60	0.99
3:C:2101:BTB:H12	3:C:2101:BTB:H62	1.65	0.79
3:A:2101:BTB:C3	7:A:5025:HOH:O	2.25	0.71
1:C:537:GLU:CD	2:C:2001:2DG:C1	2.59	0.70
1:A:537:GLU:CD	2:A:2001:2DG:C1	2.60	0.69
1:B:887:GLN:NE2	1:B:980:GLU:O	2.25	0.69
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.78	0.66
1:A:887:GLN:NE2	1:A:980:GLU:O	2.26	0.66
1:D:7:ASP:CG	1:D:8:PRO:HA	2.17	0.64
1:D:663:LEU:HD21	1:D:688:PRO:HB3	1.82	0.60
1:A:431:ARG:NH1	7:A:5005:HOH:O	2.34	0.60
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.83	0.59
1:B:537:GLU:CD	2:B:2001:2DG:C1	2.64	0.58
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.88	0.56
1:B:7:ASP:HB3	1:B:8:PRO:CA	2.36	0.56
1:A:699:ARG:NH2	7:A:4968:HOH:O	2.40	0.55
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.90	0.54
1:C:576:ILE:HG12	6:C:8008:DMS:C2	2.38	0.53
3:A:2101:BTB:H41	3:A:2101:BTB:H62	1.89	0.53
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.45	0.52
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.45	0.52
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.92	0.52
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.45	0.52
1:B:7:ASP:HB3	1:B:8:PRO:HA	1.92	0.52
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.93	0.51
1:B:7:ASP:CB	1:B:8:PRO:HA	2.41	0.51
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.46	0.51
1:C:88:SER:HA	1:C:366:VAL:HG21	1.93	0.50
1:A:7:ASP:CB	1:A:8:PRO:HA	2.42	0.50
1:B:381:GLN:O	1:B:621:LYS:HE3	2.12	0.50
1:A:7:ASP:CG	1:A:8:PRO:HA	2.32	0.49
1:D:88:SER:HA	1:D:366:VAL:HG21	1.93	0.49
3:A:2101:BTB:H62	3:A:2101:BTB:C4	2.42	0.49
1:C:755:ARG:HB3	1:C:769:TRP:HB2	1.95	0.49
1:D:749:ILE:HD13	1:D:858:ILE:HD12	1.95	0.49
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.94	0.48
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.94	0.48
1:B:9:VAL:HG12	1:C:9:VAL:HG12	1.96	0.48
1:D:576:ILE:HD11	7:D:4261:HOH:O	2.14	0.48
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.95	0.48
1:D:225:PHE:HA	1:D:243:GLU:O	2.14	0.48
1:C:7:ASP:CG	1:C:8:PRO:HA	2.35	0.47
3:C:2101:BTB:H42	3:C:2101:BTB:H52	1.67	0.47
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.78	0.47
1:B:1017:GLN:HB2	7:B:4680:HOH:O	2.13	0.47
1:A:88:SER:HA	1:A:366:VAL:HG21	1.97	0.47
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.15	0.47
1:A:615:PRO:O	1:A:618:THR:HG22	2.15	0.47
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.50	0.46
1:C:147:ASN:HA	1:C:148:SER:HA	1.68	0.46
1:C:362:LEU:HG	1:C:576:ILE:HD12	1.97	0.46
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.50	0.46
1:D:1017:GLN:HB2	7:D:4859:HOH:O	2.16	0.46
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.45
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.51	0.45
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.45
1:B:427:THR:HG21	1:B:462:SER:HB3	1.99	0.45
1:A:794:ALA:HA	1:A:998:SER:O	2.17	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.68	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.72	0.44
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.52	0.44
1:D:896:ASN:HB3	1:D:945:ASN:HB2	1.99	0.44
1:A:301:TRP:CH2	1:A:452:SER:HA	2.52	0.44
1:A:625:GLN:NE2	7:A:4190:HOH:O	2.50	0.43
1:C:143:PHE:O	1:C:168:PRO:HA	2.19	0.43
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.43
1:D:804:ASN:O	1:D:1001:PRO:HG3	2.18	0.43
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.18	0.43
1:B:545:SER:O	1:B:909:ARG:HD3	2.19	0.43
1:D:52:ARG:NH2	7:D:4628:HOH:O	2.51	0.43
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.54	0.43
1:C:724:GLU:O	1:D:847:LYS:NZ	2.52	0.42
3:A:2101:BTB:H52	3:A:2101:BTB:H32	1.62	0.42
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	2.00	0.42
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.99	0.42
1:B:279:ILE:HD11	1:C:424:ASN:OD1	2.19	0.42
1:C:750:GLU:HG3	1:C:755:ARG:HD2	2.02	0.42
1:D:755:ARG:HB2	1:D:769:TRP:HB2	2.00	0.42
1:B:674:PRO:O	1:B:675:GLN:HB2	2.20	0.42
1:A:738:PRO:HG2	1:A:834:VAL:HG23	2.02	0.42
1:D:360:HIS:HE1	1:D:362:LEU:HD12	1.84	0.42
1:D:739:HIS:HB2	7:D:4732:HOH:O	2.20	0.42
1:D:372:MET:HE1	1:D:395:HIS:HB3	2.01	0.42
3:B:2101:BTB:H12	3:B:2101:BTB:H71	1.89	0.41
1:D:615:PRO:O	1:D:618:THR:HG22	2.19	0.41
1:D:888:LEU:O	1:D:981:GLY:HA3	2.20	0.41
1:A:372:MET:HE1	1:A:395:HIS:HB3	2.02	0.41
1:B:153:TRP:HB2	1:B:185:ALA:HB3	2.01	0.41
1:C:763:GLY:HA3	1:C:822:LEU:HD13	2.01	0.41
1:B:19:PRO:HD3	1:B:112:PRO:CB	2.51	0.41
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.56	0.41
1:B:890:GLN:HB2	7:B:4683:HOH:O	2.21	0.41
3:B:2101:BTB:H32	3:B:2101:BTB:H52	1.97	0.41
1:D:843:GLN:HA	1:D:847:LYS:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.03	0.41
1:C:793:ILE:HA	1:C:807:VAL:HG11	2.02	0.41
1:B:181:GLU:HG2	7:B:4842:HOH:O	2.20	0.41
1:B:749:ILE:HD13	1:B:858:ILE:HD12	2.02	0.41
1:C:847:LYS:NZ	1:D:724:GLU:O	2.54	0.41
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.55	0.40
1:C:340:GLY:O	1:C:561:ARG:HG2	2.21	0.40
1:D:768:MET:HB2	1:D:768:MET:HE3	1.84	0.40
1:A:225:PHE:HA	1:A:243:GLU:O	2.21	0.40
1:B:13:ARG:HD3	1:B:13:ARG:HA	1.89	0.40
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.40
1:C:377:LEU:HD22	1:C:708:TRP:HA	2.03	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	1017/1052 (97%)	989 (97%)	27 (3%)	1 (0%)	51	54
1	B	1016/1052 (97%)	984 (97%)	31 (3%)	1 (0%)	51	54
1	C	1016/1052 (97%)	982 (97%)	33 (3%)	1 (0%)	51	54
1	D	1016/1052 (97%)	981 (97%)	34 (3%)	1 (0%)	51	54
All	All	4065/4208 (97%)	3936 (97%)	125 (3%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	PRO
1	D	8	PRO
1	A	8	PRO

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Mol	Chain	Res	Type
1	C	8	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	872/898 (97%)	865 (99%)	7 (1%)	81 86
1	B	871/898 (97%)	863 (99%)	8 (1%)	78 84
1	C	871/898 (97%)	865 (99%)	6 (1%)	84 88
1	D	871/898 (97%)	865 (99%)	6 (1%)	84 88
All	All	3485/3592 (97%)	3458 (99%)	27 (1%)	81 86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	PRO
1	A	333	ARG
1	A	344	LEU
1	A	546	LEU
1	A	772	ASP
1	A	956	GLN
1	B	7	ASP
1	B	80	GLU
1	B	262	GLN
1	B	333	ARG
1	B	344	LEU
1	B	546	LEU
1	B	850	PHE
1	B	956	GLN
1	C	7	ASP
1	C	267	VAL
1	C	333	ARG
1	C	546	LEU
1	C	956	GLN

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Mol	Chain	Res	Type
1	C	1017	GLN
1	D	7	ASP
1	D	333	ARG
1	D	344	LEU
1	D	546	LEU
1	D	687	GLN
1	D	956	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	890	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 123 ligands modelled in this entry, 25 are monoatomic - leaving 98 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	$\#\|Z\| > 2$
6	DMS	D	8019	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DMS	B	8023	-	3,3,3	2.65	1 (33%)	3,3,3	0.67	0
6	DMS	B	8008	-	3,3,3	2.60	1 (33%)	3,3,3	0.51	0
6	DMS	C	8005	-	3,3,3	2.63	1 (33%)	3,3,3	0.55	0
6	DMS	D	8020	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
6	DMS	C	8014	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
6	DMS	D	8012	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
6	DMS	D	8006	-	3,3,3	2.60	1 (33%)	3,3,3	0.36	0
6	DMS	A	8007	-	3,3,3	2.61	1 (33%)	3,3,3	0.51	0
6	DMS	C	8012	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
6	DMS	B	8013	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
6	DMS	B	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
6	DMS	C	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
6	DMS	C	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
6	DMS	B	8009	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
6	DMS	B	8005	-	3,3,3	2.63	1 (33%)	3,3,3	0.42	0
6	DMS	B	8024	-	3,3,3	2.57	1 (33%)	3,3,3	0.54	0
6	DMS	D	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.44	0
6	DMS	A	8012	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
6	DMS	C	8023	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
6	DMS	A	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
6	DMS	A	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
6	DMS	D	8002	-	3,3,3	2.52	1 (33%)	3,3,3	0.40	0
6	DMS	D	8022	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
6	DMS	B	8002	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
6	DMS	B	8010	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
6	DMS	A	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
6	DMS	C	8011	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
6	DMS	D	8007	-	3,3,3	2.60	1 (33%)	3,3,3	0.38	0
6	DMS	A	8005	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
6	DMS	A	8015	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
6	DMS	D	8001	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
3	BTB	D	2101	-	13,13,13	0.47	0	7,16,16	0.39	0
6	DMS	C	8006	-	3,3,3	2.59	1 (33%)	3,3,3	0.38	0
6	DMS	B	8011	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
6	DMS	C	8004	-	3,3,3	2.59	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DMS	C	8003	-	3,3,3	2.60	1 (33%)	3,3,3	0.52	0
6	DMS	D	8021	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
6	DMS	B	8016	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
6	DMS	C	8009	-	3,3,3	2.58	1 (33%)	3,3,3	0.58	0
6	DMS	D	8009	-	3,3,3	2.61	1 (33%)	3,3,3	0.44	0
6	DMS	B	8018	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
6	DMS	A	8002	-	3,3,3	2.59	1 (33%)	3,3,3	0.63	0
6	DMS	C	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
3	BTB	C	2101	-	13,13,13	0.34	0	7,16,16	0.64	0
2	2DG	B	2001	1,5	10,10,11	0.34	0	13,13,15	1.17	1 (7%)
6	DMS	A	8011	-	3,3,3	2.59	1 (33%)	3,3,3	0.43	0
6	DMS	C	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
6	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.53	0
6	DMS	A	8003	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
6	DMS	B	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.54	0
6	DMS	B	8020	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
6	DMS	D	8003	-	3,3,3	2.59	1 (33%)	3,3,3	0.41	0
6	DMS	B	8022	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
6	DMS	B	8007	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
6	DMS	A	8019	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
6	DMS	D	8017	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
3	BTB	A	2101	-	13,13,13	0.43	0	7,16,16	0.59	0
2	2DG	A	2001	1,5	10,10,11	0.41	0	13,13,15	1.19	1 (7%)
6	DMS	C	8021	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
6	DMS	B	8021	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
6	DMS	B	8012	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
6	DMS	D	8018	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
6	DMS	C	8022	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
6	DMS	C	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
6	DMS	B	8006	-	3,3,3	2.62	1 (33%)	3,3,3	0.44	0
6	DMS	D	8013	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
6	DMS	D	8010	-	3,3,3	2.62	1 (33%)	3,3,3	0.51	0
2	2DG	C	2001	1,5	10,10,11	0.35	0	13,13,15	1.20	2 (15%)
6	DMS	A	8006	-	3,3,3	2.58	1 (33%)	3,3,3	0.27	0
6	DMS	D	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DMS	C	8015	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
6	DMS	C	8024	-	3,3,3	2.63	1 (33%)	3,3,3	0.55	0
6	DMS	B	8014	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
6	DMS	C	8025	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
3	BTB	B	2101	-	13,13,13	0.52	0	7,16,16	0.83	0
6	DMS	B	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
6	DMS	C	8002	-	3,3,3	2.57	1 (33%)	3,3,3	0.43	0
6	DMS	A	8014	-	3,3,3	2.61	1 (33%)	3,3,3	0.43	0
6	DMS	C	8016	-	3,3,3	2.64	1 (33%)	3,3,3	0.45	0
6	DMS	B	8003	-	3,3,3	2.58	1 (33%)	3,3,3	0.44	0
6	DMS	B	8015	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
6	DMS	D	8008	-	3,3,3	2.65	1 (33%)	3,3,3	0.43	0
6	DMS	A	8009	-	3,3,3	2.58	1 (33%)	3,3,3	0.43	0
6	DMS	D	8011	-	3,3,3	2.60	1 (33%)	3,3,3	0.42	0
6	DMS	B	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
6	DMS	A	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
6	DMS	C	8008	-	3,3,3	2.60	1 (33%)	3,3,3	0.50	0
6	DMS	A	8016	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
6	DMS	A	8018	-	3,3,3	2.61	1 (33%)	3,3,3	0.42	0
6	DMS	D	8016	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
6	DMS	C	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
2	2DG	D	2001	1,5	10,10,11	0.41	0	13,13,15	0.86	1 (7%)
6	DMS	D	8004	-	3,3,3	2.59	1 (33%)	3,3,3	0.47	0
6	DMS	D	8015	-	3,3,3	2.65	1 (33%)	3,3,3	0.41	0
6	DMS	A	8008	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
6	DMS	C	8018	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
6	DMS	C	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	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
3	BTB	D	2101	-	-	3/21/21/21	-
2	2DG	C	2001	1,5	-	1/2/16/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTB	B	2101	-	-	2/21/21/21	-
3	BTB	A	2101	-	-	3/21/21/21	-
3	BTB	C	2101	-	-	3/21/21/21	-
2	2DG	D	2001	1,5	-	1/2/16/18	0/1/1/1
2	2DG	A	2001	1,5	-	1/2/16/18	0/1/1/1
2	2DG	B	2001	1,5	-	1/2/16/18	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8017	DMS	O-S	4.53	1.80	1.50
6	B	8012	DMS	O-S	4.51	1.80	1.50
6	D	8020	DMS	O-S	4.51	1.80	1.50
6	C	8001	DMS	O-S	4.51	1.80	1.50
6	D	8018	DMS	O-S	4.51	1.80	1.50
6	C	8018	DMS	O-S	4.50	1.80	1.50
6	C	8011	DMS	O-S	4.50	1.80	1.50
6	B	8007	DMS	O-S	4.50	1.80	1.50
6	A	8008	DMS	O-S	4.49	1.80	1.50
6	D	8001	DMS	O-S	4.49	1.80	1.50
6	C	8012	DMS	O-S	4.49	1.80	1.50
6	B	8011	DMS	O-S	4.49	1.80	1.50
6	B	8022	DMS	O-S	4.48	1.80	1.50
6	D	8021	DMS	O-S	4.48	1.80	1.50
6	B	8001	DMS	O-S	4.47	1.80	1.50
6	D	8016	DMS	O-S	4.47	1.80	1.50
6	C	8007	DMS	O-S	4.47	1.80	1.50
6	B	8019	DMS	O-S	4.47	1.80	1.50
6	D	8012	DMS	O-S	4.46	1.80	1.50
6	C	8020	DMS	O-S	4.46	1.80	1.50
6	C	8023	DMS	O-S	4.46	1.80	1.50
6	C	8010	DMS	O-S	4.46	1.80	1.50
6	A	8001	DMS	O-S	4.46	1.80	1.50
6	A	8017	DMS	O-S	4.46	1.80	1.50
6	C	8015	DMS	O-S	4.46	1.80	1.50
6	C	8014	DMS	O-S	4.46	1.80	1.50
6	B	8015	DMS	O-S	4.46	1.80	1.50
6	B	8017	DMS	O-S	4.46	1.80	1.50
6	B	8014	DMS	O-S	4.46	1.80	1.50
6	A	8012	DMS	O-S	4.46	1.80	1.50
6	B	8020	DMS	O-S	4.46	1.80	1.50
6	D	8022	DMS	O-S	4.45	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	8021	DMS	O-S	4.45	1.80	1.50
6	A	8013	DMS	O-S	4.45	1.80	1.50
6	B	8023	DMS	O-S	4.45	1.80	1.50
6	C	8019	DMS	O-S	4.45	1.80	1.50
6	D	8015	DMS	O-S	4.45	1.80	1.50
6	D	8008	DMS	O-S	4.45	1.80	1.50
6	B	8009	DMS	O-S	4.45	1.80	1.50
6	A	8015	DMS	O-S	4.44	1.80	1.50
6	D	8019	DMS	O-S	4.44	1.80	1.50
6	C	8013	DMS	O-S	4.44	1.80	1.50
6	D	8014	DMS	O-S	4.44	1.80	1.50
6	A	8005	DMS	O-S	4.44	1.80	1.50
6	C	8016	DMS	O-S	4.44	1.80	1.50
6	C	8017	DMS	O-S	4.44	1.80	1.50
6	A	8010	DMS	O-S	4.44	1.80	1.50
6	D	8005	DMS	O-S	4.43	1.80	1.50
6	A	8016	DMS	O-S	4.43	1.80	1.50
6	C	8025	DMS	O-S	4.43	1.80	1.50
6	B	8013	DMS	O-S	4.43	1.80	1.50
6	C	8005	DMS	O-S	4.43	1.80	1.50
6	B	8005	DMS	O-S	4.42	1.80	1.50
6	C	8022	DMS	O-S	4.42	1.80	1.50
6	A	8019	DMS	O-S	4.42	1.80	1.50
6	B	8018	DMS	O-S	4.42	1.80	1.50
6	D	8013	DMS	O-S	4.41	1.80	1.50
6	A	8014	DMS	O-S	4.41	1.80	1.50
6	C	8024	DMS	O-S	4.40	1.80	1.50
6	B	8021	DMS	O-S	4.40	1.80	1.50
6	B	8002	DMS	O-S	4.40	1.80	1.50
6	A	8018	DMS	O-S	4.39	1.79	1.50
6	B	8016	DMS	O-S	4.39	1.79	1.50
6	B	8006	DMS	O-S	4.39	1.79	1.50
6	D	8010	DMS	O-S	4.38	1.79	1.50
6	A	8003	DMS	O-S	4.38	1.79	1.50
6	A	8007	DMS	O-S	4.38	1.79	1.50
6	B	8004	DMS	O-S	4.38	1.79	1.50
6	D	8011	DMS	O-S	4.38	1.79	1.50
6	B	8010	DMS	O-S	4.38	1.79	1.50
6	D	8009	DMS	O-S	4.37	1.79	1.50
6	A	8004	DMS	O-S	4.37	1.79	1.50
6	C	8008	DMS	O-S	4.35	1.79	1.50
6	C	8003	DMS	O-S	4.35	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8006	DMS	O-S	4.35	1.79	1.50
6	D	8007	DMS	O-S	4.35	1.79	1.50
6	C	8004	DMS	O-S	4.35	1.79	1.50
6	C	8006	DMS	O-S	4.35	1.79	1.50
6	B	8008	DMS	O-S	4.35	1.79	1.50
6	D	8004	DMS	O-S	4.34	1.79	1.50
6	D	8003	DMS	O-S	4.34	1.79	1.50
6	A	8011	DMS	O-S	4.34	1.79	1.50
6	B	8003	DMS	O-S	4.33	1.79	1.50
6	A	8002	DMS	O-S	4.32	1.79	1.50
6	A	8006	DMS	O-S	4.32	1.79	1.50
6	C	8002	DMS	O-S	4.32	1.79	1.50
6	C	8009	DMS	O-S	4.32	1.79	1.50
6	A	8009	DMS	O-S	4.31	1.79	1.50
6	B	8024	DMS	O-S	4.29	1.79	1.50
6	D	8002	DMS	O-S	4.22	1.78	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	2DG	C1-O5-C5	3.65	118.36	112.01
2	C	2001	2DG	C1-O5-C5	3.31	117.77	112.01
2	A	2001	2DG	C1-O5-C5	3.30	117.75	112.01
2	D	2001	2DG	C1-O5-C5	2.46	116.29	112.01
2	C	2001	2DG	O5-C1-C2	2.29	115.11	110.73

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2101	BTB	O1-C1-C2-C3
3	A	2101	BTB	O1-C1-C2-C4
3	A	2101	BTB	O1-C1-C2-N
2	A	2001	2DG	O5-C5-C6-O6
2	B	2001	2DG	O5-C5-C6-O6
2	D	2001	2DG	O5-C5-C6-O6
2	C	2001	2DG	O5-C5-C6-O6
3	B	2101	BTB	N-C7-C8-O8
3	B	2101	BTB	O1-C1-C2-N
3	C	2101	BTB	N-C2-C3-O3
3	D	2101	BTB	O1-C1-C2-N
3	C	2101	BTB	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	2101	BTB	C4-C2-C3-O3
3	D	2101	BTB	O1-C1-C2-C3
3	D	2101	BTB	O1-C1-C2-C4

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2101	BTB	2	0
2	B	2001	2DG	1	0
3	A	2101	BTB	5	0
2	A	2001	2DG	1	0
2	C	2001	2DG	1	0
3	B	2101	BTB	2	0
6	C	8008	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	1019/1052 (96%)	-0.45	19 (1%)	66	71	14, 26, 50, 91	0
1	B	1018/1052 (96%)	-0.41	14 (1%)	75	78	15, 28, 53, 91	0
1	C	1018/1052 (96%)	-0.44	18 (1%)	68	72	14, 28, 53, 98	0
1	D	1018/1052 (96%)	-0.40	19 (1%)	66	71	14, 27, 52, 94	0
All	All	4073/4208 (96%)	-0.43	70 (1%)	70	74	14, 27, 52, 98	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	PRO	7.5
1	D	689	GLU	6.8
1	B	8	PRO	6.4
1	A	6	ILE	6.1
1	C	689	GLU	6.1
1	D	8	PRO	6.1
1	D	7	ASP	5.5
1	B	689	GLU	5.5
1	C	8	PRO	5.5
1	A	5	MET	5.4
1	C	6	ILE	5.2
1	D	6	ILE	4.8
1	C	7	ASP	4.7
1	B	731	PRO	4.5
1	B	732	ALA	4.4
1	A	7	ASP	4.4
1	A	689	GLU	4.3
1	A	735	HIS	4.2
1	A	732	ALA	3.9
1	C	733	ALA	3.9
1	C	730	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	735	HIS	3.8
1	A	686	PRO	3.8
1	A	799	THR	3.7
1	A	1023	LYS	3.7
1	D	731	PRO	3.5
1	B	799	THR	3.4
1	B	687	GLN	3.3
1	A	731	PRO	3.3
1	C	11	LEU	3.3
1	C	745	MET	3.2
1	D	732	ALA	3.1
1	A	687	GLN	3.1
1	D	687	GLN	3.1
1	D	733	ALA	3.1
1	B	6	ILE	3.0
1	D	12	GLN	3.0
1	A	685	LEU	3.0
1	C	731	PRO	3.0
1	D	1023	LYS	2.9
1	D	11	LEU	2.9
1	D	686	PRO	2.9
1	A	11	LEU	2.9
1	D	179	ALA	2.9
1	B	733	ALA	2.8
1	B	11	LEU	2.8
1	B	12	GLN	2.8
1	B	686	PRO	2.8
1	B	7	ASP	2.7
1	A	771	GLY	2.6
1	A	12	GLN	2.6
1	C	686	PRO	2.6
1	C	684	GLU	2.5
1	C	799	THR	2.5
1	C	9	VAL	2.4
1	D	663	LEU	2.4
1	A	734	SER	2.4
1	A	772	ASP	2.4
1	C	772	ASP	2.4
1	C	687	GLN	2.3
1	D	772	ASP	2.3
1	D	730	LEU	2.3
1	A	684	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	831	ALA	2.3
1	B	684	GLU	2.3
1	D	831	ALA	2.2
1	C	12	GLN	2.2
1	D	739	HIS	2.1
1	B	730	LEU	2.1
1	C	685	LEU	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, 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
6	DMS	D	8020	4/4	0.68	0.25	73,73,76,79	0
6	DMS	C	8025	4/4	0.72	0.29	71,74,75,77	0
6	DMS	C	8019	4/4	0.78	0.30	66,68,70,73	0
6	DMS	C	8001	4/4	0.79	0.19	47,56,57,64	0
6	DMS	B	8022	4/4	0.80	0.26	80,81,81,82	0
6	DMS	B	8012	4/4	0.80	0.26	61,63,63,72	0
6	DMS	C	8014	4/4	0.80	0.25	73,74,75,77	0
6	DMS	D	8017	4/4	0.83	0.16	69,70,70,73	0
6	DMS	B	8002	4/4	0.83	0.26	68,69,70,72	0
6	DMS	C	8011	4/4	0.85	0.20	60,62,65,65	0
6	DMS	C	8024	4/4	0.86	0.20	64,65,67,68	0
5	NA	C	3104	1/1	0.86	0.11	42,42,42,42	0
6	DMS	D	8019	4/4	0.87	0.33	80,80,81,82	0
6	DMS	B	8019	4/4	0.88	0.12	70,72,72,74	0
5	NA	C	3103	1/1	0.88	0.20	38,38,38,38	0
6	DMS	D	8018	4/4	0.88	0.23	64,64,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	B	8023	4/4	0.88	0.24	56,61,62,64	0
6	DMS	A	8012	4/4	0.88	0.21	75,77,77,77	0
6	DMS	B	8014	4/4	0.89	0.20	60,61,63,64	0
6	DMS	D	8001	4/4	0.89	0.15	55,55,58,63	0
6	DMS	C	8018	4/4	0.89	0.18	83,83,83,84	0
6	DMS	B	8021	4/4	0.89	0.20	56,60,61,63	0
6	DMS	C	8022	4/4	0.89	0.27	57,63,64,67	0
6	DMS	B	8017	4/4	0.89	0.18	63,65,69,69	0
6	DMS	D	8021	4/4	0.89	0.17	76,77,77,79	0
6	DMS	D	8013	4/4	0.90	0.21	80,80,82,82	0
6	DMS	D	8015	4/4	0.90	0.18	69,70,70,71	0
6	DMS	A	8001	4/4	0.90	0.12	53,54,55,58	0
6	DMS	B	8020	4/4	0.90	0.20	68,72,72,74	0
6	DMS	A	8018	4/4	0.90	0.30	64,67,69,70	0
6	DMS	C	8005	4/4	0.90	0.18	50,51,54,55	0
6	DMS	D	8012	4/4	0.90	0.14	42,46,50,54	0
6	DMS	C	8012	4/4	0.91	0.16	63,64,66,68	0
6	DMS	C	8013	4/4	0.91	0.18	70,70,71,73	0
5	NA	A	3104	1/1	0.91	0.14	45,45,45,45	0
6	DMS	C	8015	4/4	0.91	0.16	67,68,68,69	0
6	DMS	A	8017	4/4	0.91	0.16	65,67,69,72	0
3	BTB	C	2101	14/14	0.91	0.14	26,36,41,54	0
6	DMS	C	8021	4/4	0.92	0.16	73,74,75,76	0
6	DMS	B	8018	4/4	0.92	0.16	61,62,63,64	0
6	DMS	B	8005	4/4	0.92	0.13	46,49,53,54	0
4	MG	D	3002	1/1	0.92	0.09	24,24,24,24	0
6	DMS	A	8007	4/4	0.92	0.15	62,63,65,65	0
6	DMS	D	8011	4/4	0.92	0.30	60,63,63,63	0
3	BTB	D	2101	14/14	0.92	0.14	30,33,43,53	0
6	DMS	D	8022	4/4	0.92	0.17	67,68,70,71	0
6	DMS	C	8020	4/4	0.93	0.21	60,61,64,65	0
6	DMS	B	8010	4/4	0.93	0.18	44,49,52,53	0
3	BTB	B	2101	14/14	0.93	0.13	25,34,42,54	0
6	DMS	C	8023	4/4	0.93	0.12	52,55,56,58	0
6	DMS	A	8016	4/4	0.93	0.21	67,68,68,69	0
6	DMS	C	8016	4/4	0.93	0.10	47,50,54,56	0
6	DMS	B	8015	4/4	0.93	0.20	75,76,76,77	0
6	DMS	D	8005	4/4	0.93	0.15	49,52,55,58	0
6	DMS	A	8010	4/4	0.93	0.15	43,44,48,49	0
6	DMS	B	8001	4/4	0.94	0.25	56,57,57,62	0
6	DMS	C	8017	4/4	0.94	0.18	67,67,68,69	0
6	DMS	B	8013	4/4	0.94	0.16	67,68,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BTB	A	2101	14/14	0.94	0.14	19,36,42,52	0
6	DMS	D	8003	4/4	0.94	0.16	30,38,39,39	0
4	MG	B	3001	1/1	0.94	0.09	23,23,23,23	0
5	NA	B	3102	1/1	0.94	0.08	24,24,24,24	0
6	DMS	B	8011	4/4	0.94	0.13	68,69,70,70	0
6	DMS	A	8014	4/4	0.95	0.10	38,45,47,50	0
4	MG	C	3002	1/1	0.95	0.07	28,28,28,28	0
6	DMS	A	8003	4/4	0.95	0.13	31,37,40,43	0
6	DMS	A	8005	4/4	0.95	0.14	53,56,58,60	0
5	NA	A	3103	1/1	0.95	0.08	33,33,33,33	0
5	NA	D	3101	1/1	0.95	0.09	21,21,21,21	0
6	DMS	B	8016	4/4	0.95	0.15	61,61,63,63	0
6	DMS	C	8003	4/4	0.95	0.11	22,34,34,35	0
5	NA	D	3104	1/1	0.95	0.10	44,44,44,44	0
6	DMS	D	8007	4/4	0.95	0.16	49,52,53,53	0
5	NA	D	3103	1/1	0.96	0.15	32,32,32,32	0
6	DMS	D	8014	4/4	0.96	0.17	68,69,69,70	0
6	DMS	A	8011	4/4	0.96	0.10	42,46,47,47	0
6	DMS	D	8016	4/4	0.96	0.16	41,49,49,50	0
2	2DG	C	2001	10/11	0.96	0.10	13,19,21,23	0
5	NA	B	3104	1/1	0.96	0.16	40,40,40,40	0
5	NA	A	3102	1/1	0.96	0.13	22,22,22,22	0
4	MG	A	3002	1/1	0.96	0.10	22,22,22,22	0
4	MG	D	3001	1/1	0.96	0.04	24,24,24,24	0
6	DMS	A	8008	4/4	0.96	0.11	41,41,44,46	0
4	MG	C	3001	1/1	0.97	0.07	22,22,22,22	0
5	NA	C	3101	1/1	0.97	0.07	22,22,22,22	0
6	DMS	D	8006	4/4	0.97	0.12	39,39,42,43	0
6	DMS	B	8006	4/4	0.97	0.12	46,46,46,46	0
6	DMS	D	8010	4/4	0.97	0.11	47,48,48,49	0
6	DMS	B	8008	4/4	0.97	0.12	36,39,40,41	0
6	DMS	A	8013	4/4	0.97	0.12	64,65,65,66	0
5	NA	C	3102	1/1	0.97	0.12	22,22,22,22	0
2	2DG	B	2001	10/11	0.97	0.10	13,17,20,21	0
6	DMS	B	8024	4/4	0.97	0.11	23,30,31,33	0
2	2DG	A	2001	10/11	0.97	0.09	15,17,20,20	0
5	NA	B	3101	1/1	0.97	0.07	23,23,23,23	0
6	DMS	A	8019	4/4	0.97	0.13	62,63,63,64	0
6	DMS	C	8008	4/4	0.97	0.15	44,44,46,53	0
6	DMS	C	8009	4/4	0.97	0.13	34,41,41,44	0
6	DMS	C	8010	4/4	0.97	0.17	51,54,56,56	0
4	MG	B	3003	1/1	0.97	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	D	8008	4/4	0.98	0.10	45,48,49,50	0
6	DMS	D	8009	4/4	0.98	0.14	43,45,45,49	0
6	DMS	C	8007	4/4	0.98	0.11	46,49,49,51	0
4	MG	B	3002	1/1	0.98	0.09	26,26,26,26	0
6	DMS	A	8015	4/4	0.98	0.16	62,62,63,64	0
6	DMS	B	8007	4/4	0.98	0.10	43,43,46,46	0
5	NA	B	3103	1/1	0.98	0.09	34,34,34,34	0
6	DMS	A	8009	4/4	0.98	0.17	41,43,44,46	0
6	DMS	A	8002	4/4	0.98	0.12	24,25,27,29	0
5	NA	D	3102	1/1	0.98	0.09	24,24,24,24	0
6	DMS	D	8002	4/4	0.98	0.09	23,26,27,34	0
5	NA	A	3101	1/1	0.98	0.09	23,23,23,23	0
6	DMS	A	8006	4/4	0.98	0.11	36,36,37,37	0
6	DMS	B	8003	4/4	0.98	0.11	29,31,31,33	0
6	DMS	B	8004	4/4	0.98	0.14	39,40,41,44	0
6	DMS	A	8004	4/4	0.99	0.10	35,38,40,42	0
6	DMS	C	8004	4/4	0.99	0.09	32,35,35,36	0
4	MG	A	3001	1/1	0.99	0.05	19,19,19,19	0
6	DMS	C	8006	4/4	0.99	0.10	40,40,40,41	0
2	2DG	D	2001	10/11	0.99	0.09	15,17,20,22	0
6	DMS	D	8004	4/4	0.99	0.12	36,36,36,36	0
6	DMS	B	8009	4/4	0.99	0.11	44,45,46,46	0
6	DMS	C	8002	4/4	0.99	0.11	29,30,31,35	0

6.5 Other polymers (i)

There are no such residues in this entry.