Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:07 AM BST

PDB ID	:	3T09
Title	:	E. coli (LacZ) beta-galactosidase (S796A) galactonolactone complex
Authors	:	Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.
Deposited on	:	2011-07-19
Resolution	:	1.75 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

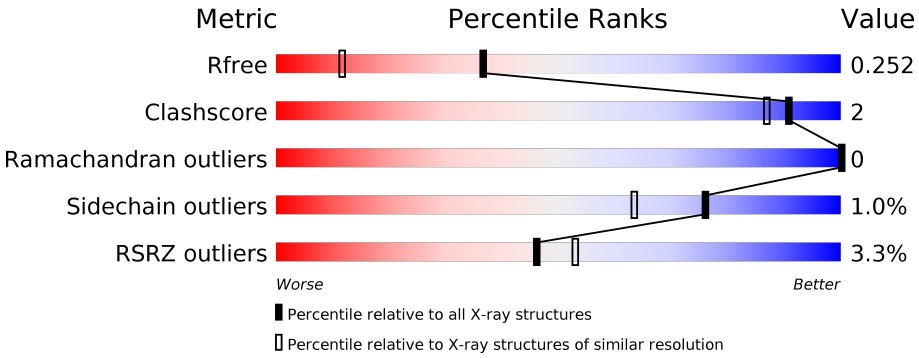
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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	3% 92%
1	B	1052	2% 91% 6%
1	C	1052	3% 91% 5%
1	D	1052	4% 92%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	B	8007	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37438 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			
1	B	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			
1	C	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			
1	D	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	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	796	ALA	SER	engineered mutation	UNP P00722
B	-28	MET	-	expression tag	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	796	ALA	SER	engineered mutation	UNP P00722
C	-28	MET	-	expression tag	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	796	ALA	SER	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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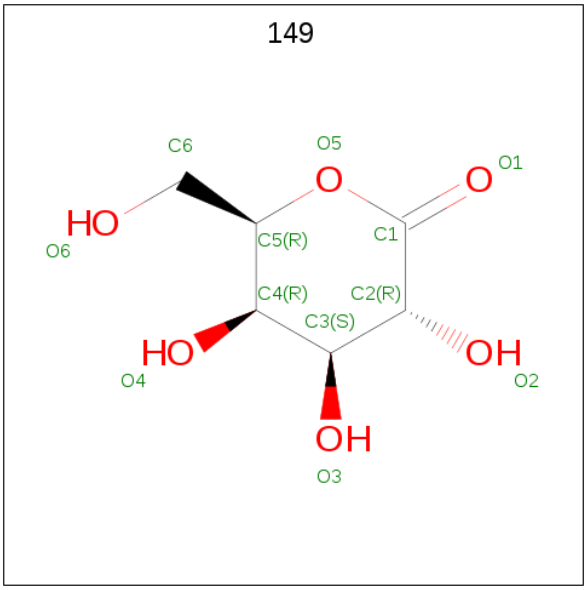
Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	796	ALA	SER	engineered mutation	UNP P00722

- Molecule 2 is D-galactonolactone (three-letter code: 149) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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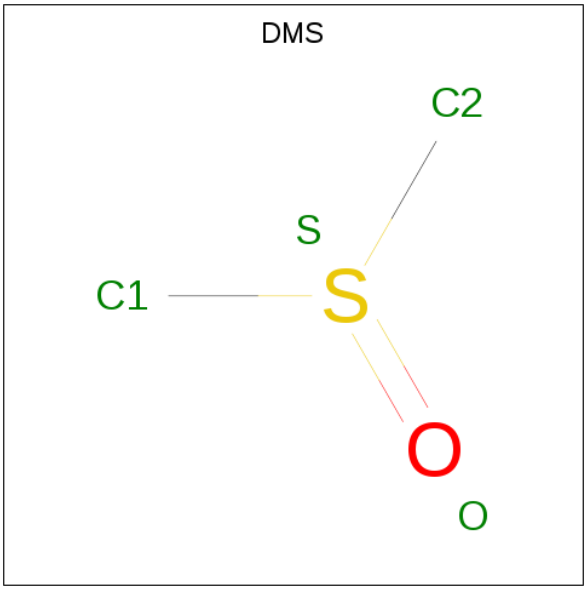
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

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

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

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



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

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

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

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

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

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

- Molecule 6 is water.

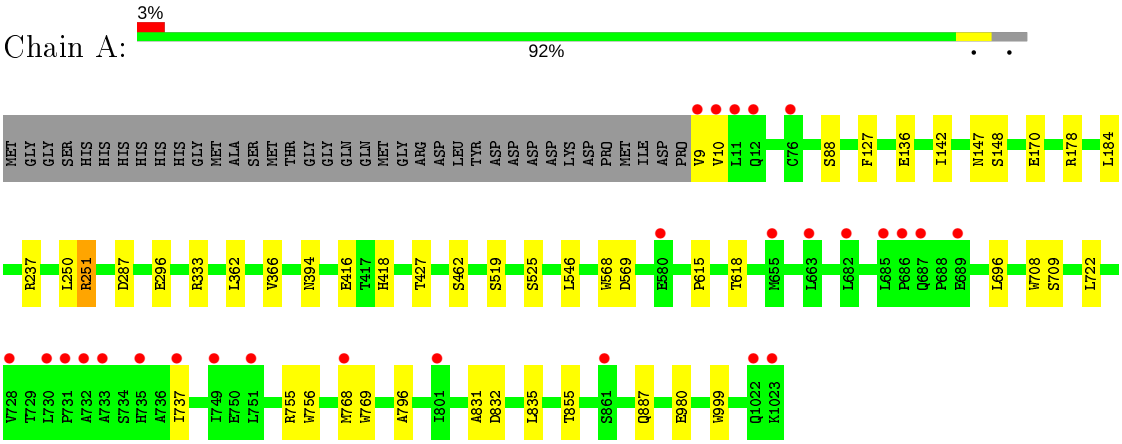
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1092	Total O 1092 1092	0	0
6	B	1047	Total O 1047 1047	0	0
6	C	1073	Total O 1073 1073	0	0
6	D	1099	Total O 1099 1099	0	0

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.

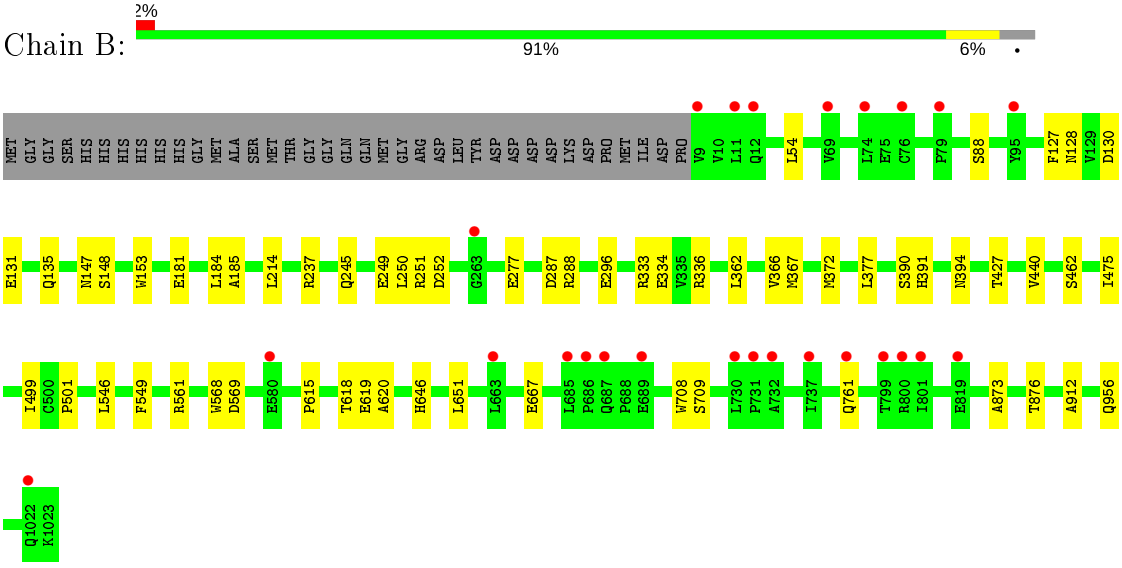
- Molecule 1: Beta-galactosidase

Chain A:



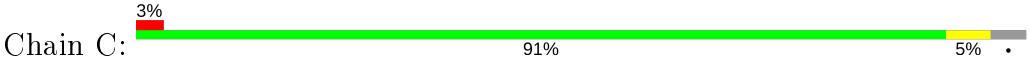
- Molecule 1: Beta-galactosidase

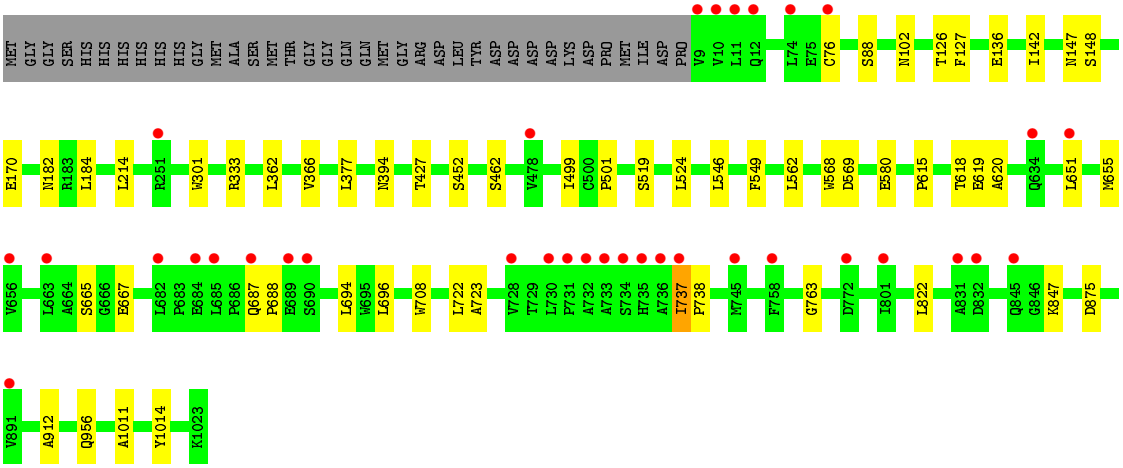
Chain B:



- Molecule 1: Beta-galactosidase

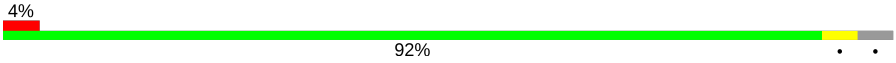
Chain C:

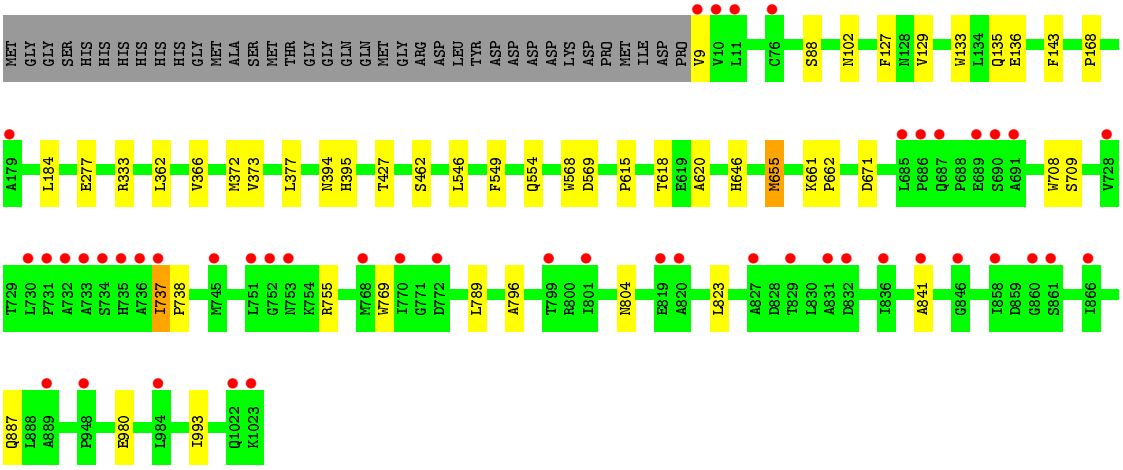




- Molecule 1: Beta-galactosidase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.88Å 151.20Å 131.81Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	128.40 – 1.75 128.40 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (128.40-1.75) 91.7 (128.40-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.215 , 0.254 0.213 , 0.252	Depositor DCC
R_{free} test set	22222 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	37438	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS, 149

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	0.38	0/8398	0.54	0/11457
1	B	0.36	0/8398	0.53	0/11457
1	C	0.36	0/8398	0.52	0/11457
1	D	0.38	0/8398	0.53	0/11457
All	All	0.37	0/33592	0.53	0/45828

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

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	8156	0	7753	28	0
1	B	8156	0	7753	30	0
1	C	8156	0	7753	27	0
1	D	8156	0	7753	28	0
2	A	12	0	9	0	0
2	B	12	0	9	1	0
2	C	12	0	9	0	0
2	D	12	0	9	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	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	116	0	174	0	0
5	B	112	0	168	1	0
5	C	100	0	150	3	0
5	D	100	0	150	3	0
6	A	1092	0	0	0	0
6	B	1047	0	0	3	0
6	C	1073	0	0	3	0
6	D	1099	0	0	2	0
All	All	37438	0	31690	112	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 (112) 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:A:251:ARG:HH11	1:A:251:ARG:CG	1.89	0.84
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.56	0.69
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.56	0.69
1:A:251:ARG:HG3	1:A:251:ARG:NH1	2.08	0.68
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.31	0.65
1:D:277:GLU:OE1	6:D:4820:HOH:O	2.15	0.63
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.81	0.62
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.64	0.62
1:B:54:LEU:HD11	1:B:214:LEU:HD13	1.81	0.62
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.34	0.62
1:A:9:VAL:HG12	1:D:9:VAL:HG12	1.83	0.58
1:B:367:MET:HE2	1:B:372:MET:HG3	1.85	0.58
1:B:131:GLU:O	1:B:135:GLN:HG2	2.05	0.56
1:B:88:SER:HA	1:B:366:VAL:HG21	1.88	0.56
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.88	0.55
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.71	0.55
1:C:847:LYS:HZ3	1:C:875:ASP:CG	2.11	0.54
1:A:427:THR:HG21	1:A:462:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG12	1:D:9:VAL:CG1	2.39	0.53
1:B:181:GLU:HG3	6:B:4914:HOH:O	2.08	0.53
1:D:655:MET:CE	1:D:662:PRO:HB3	2.38	0.53
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.90	0.53
1:C:102:ASN:HD21	5:C:8025:DMS:C1	2.22	0.53
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.90	0.53
1:D:737:ILE:HG13	1:D:738:PRO:N	2.25	0.52
1:B:873:ALA:O	1:B:876:THR:HG22	2.10	0.52
1:C:102:ASN:HD21	5:C:8025:DMS:H12	1.73	0.51
1:C:615:PRO:O	1:C:618:THR:HG22	2.10	0.51
1:A:737:ILE:HD12	1:A:832:ASP:HA	1.92	0.51
1:D:129:VAL:HG12	1:D:133:TRP:HB2	1.91	0.51
1:A:250:LEU:HD21	1:A:287:ASP:HA	1.92	0.51
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.46	0.51
1:B:651:LEU:HD21	1:B:667:GLU:HB2	1.94	0.50
1:D:755:ARG:HB3	1:D:769:TRP:HB2	1.94	0.50
1:A:887:GLN:NE2	1:A:980:GLU:O	2.37	0.49
1:B:249:GLU:HG2	1:B:251:ARG:NH1	2.27	0.49
1:B:252:ASP:HB3	6:B:4920:HOH:O	2.12	0.49
1:A:755:ARG:HB3	1:A:769:TRP:HB2	1.94	0.48
5:C:8025:DMS:H11	6:C:4922:HOH:O	2.12	0.48
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.96	0.48
1:D:887:GLN:NE2	1:D:980:GLU:O	2.43	0.48
1:C:651:LEU:HD21	1:C:667:GLU:HB2	1.95	0.48
1:B:615:PRO:O	1:B:618:THR:HG22	2.14	0.47
1:C:301:TRP:CH2	1:C:452:SER:HA	2.49	0.47
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.42	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.48	0.47
1:D:102:ASN:HD21	5:D:8024:DMS:C2	2.27	0.47
1:B:128:ASN:HB2	1:B:181:GLU:OE1	2.15	0.47
1:D:135:GLN:NE2	6:D:5036:HOH:O	2.48	0.47
1:D:655:MET:HE1	1:D:662:PRO:HB3	1.97	0.47
1:D:789:LEU:HD11	1:D:993:ILE:HG22	1.97	0.47
1:D:373:VAL:O	1:D:377:LEU:HG	2.14	0.47
1:D:88:SER:HA	1:D:366:VAL:HG21	1.96	0.47
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.50	0.46
1:C:580:GLU:HG2	6:C:4934:HOH:O	2.14	0.46
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.50	0.46
1:D:615:PRO:O	1:D:618:THR:HG22	2.15	0.46
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.97	0.46
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.97	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.98	0.45
1:A:615:PRO:O	1:A:618:THR:HG22	2.17	0.45
1:C:696:LEU:HB2	1:C:722:LEU:HD11	1.99	0.45
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.52	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.71	0.45
1:B:237:ARG:HD2	1:B:296:GLU:OE1	2.17	0.45
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.99	0.44
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.52	0.44
1:C:737:ILE:HD13	1:C:738:PRO:O	2.17	0.44
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.52	0.44
1:A:9:VAL:HG23	1:A:10:VAL:N	2.33	0.44
1:C:524:LEU:HD11	1:C:562:LEU:HG	2.00	0.44
1:A:737:ILE:HD12	1:A:831:ALA:O	2.18	0.44
1:C:427:THR:HG21	1:C:462:SER:HB3	2.00	0.44
1:A:237:ARG:HD2	1:A:296:GLU:OE1	2.18	0.43
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.53	0.43
1:C:88:SER:HA	1:C:366:VAL:HG21	2.00	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.68	0.43
1:C:377:LEU:HD22	1:C:708:TRP:HA	2.00	0.43
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.01	0.43
1:A:525:SER:O	1:B:561:ARG:HD3	2.18	0.43
1:A:756:TRP:CD1	1:A:768:MET:HG2	2.54	0.43
1:B:245:GLN:HG2	1:B:288:ARG:HG2	2.01	0.43
1:B:390:SER:HA	1:B:391:HIS:HA	1.85	0.43
1:C:147:ASN:HA	1:C:148:SER:HA	1.67	0.43
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.54	0.42
1:C:76:CYS:HB3	6:C:4960:HOH:O	2.19	0.42
1:D:427:THR:HG21	1:D:462:SER:HB3	2.00	0.42
1:A:88:SER:HA	1:A:366:VAL:HG21	2.01	0.42
1:B:427:THR:HG21	1:B:462:SER:HB3	2.01	0.42
1:C:694:LEU:HD12	1:C:723:ALA:HB3	2.02	0.42
1:B:646:HIS:HD2	6:B:4823:HOH:O	2.02	0.42
1:D:143:PHE:O	1:D:168:PRO:HA	2.19	0.42
1:C:126:THR:HA	1:C:182:ASN:O	2.20	0.42
1:D:102:ASN:HD21	5:D:8024:DMS:H22	1.84	0.42
1:C:655:MET:HG3	1:C:665:SER:HB3	2.02	0.41
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.55	0.41
1:D:661:LYS:HA	1:D:662:PRO:HD2	1.93	0.41
2:B:2001:149:H62	5:B:8028:DMS:C2	2.49	0.41
1:B:153:TRP:HB2	1:B:185:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LEU:HD11	1:A:855:THR:HB	2.02	0.41
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.56	0.41
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.55	0.41
1:A:796:ALA:HB2	1:A:999:TRP:HB3	2.03	0.41
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.49	0.41
1:D:823:LEU:HD11	1:D:841:ALA:HB2	2.03	0.41
1:D:796:ALA:HB1	5:D:8024:DMS:H22	2.03	0.40
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.56	0.40
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.21	0.40
1:B:250:LEU:HD21	1:B:287:ASP:HA	2.03	0.40
1:B:440:VAL:HG13	1:B:475:ILE:HD11	2.02	0.40
1:C:687:GLN:HA	1:C:688:PRO:HD3	1.98	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	1013/1052 (96%)	984 (97%)	29 (3%)	0	100	100
1	B	1013/1052 (96%)	983 (97%)	30 (3%)	0	100	100
1	C	1013/1052 (96%)	983 (97%)	30 (3%)	0	100	100
1	D	1013/1052 (96%)	985 (97%)	28 (3%)	0	100	100
All	All	4052/4208 (96%)	3935 (97%)	117 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	867/897 (97%)	859 (99%)	8 (1%)	78	67
1	B	867/897 (97%)	859 (99%)	8 (1%)	78	67
1	C	867/897 (97%)	858 (99%)	9 (1%)	76	63
1	D	867/897 (97%)	858 (99%)	9 (1%)	76	63
All	All	3468/3588 (97%)	3434 (99%)	34 (1%)	76	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	178	ARG
1	A	251	ARG
1	A	333	ARG
1	A	362	LEU
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	B	130	ASP
1	B	277	GLU
1	B	333	ARG
1	B	362	LEU
1	B	394	ASN
1	B	546	LEU
1	B	761	GLN
1	B	956	GLN
1	C	136	GLU
1	C	214	LEU
1	C	333	ARG
1	C	362	LEU
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	737	ILE
1	C	956	GLN
1	D	136	GLU
1	D	333	ARG
1	D	362	LEU

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Mol	Chain	Res	Type
1	D	394	ASN
1	D	546	LEU
1	D	554	GLN
1	D	655	MET
1	D	737	ILE
1	D	804	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	394	ASN
1	A	485	GLN
1	A	646	HIS
1	C	102	ASN
1	D	102	ASN
1	D	844	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 138 ligands modelled in this entry, 27 are monoatomic - leaving 111 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	8015	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
5	DMS	D	8020	4	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
5	DMS	B	8024	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
5	DMS	C	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
5	DMS	B	8009	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
5	DMS	C	8019	4	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
5	DMS	C	8002	-	3,3,3	2.59	1 (33%)	3,3,3	0.41	0
2	149	D	2001	4	12,12,12	2.30	2 (16%)	15,17,17	1.19	2 (13%)
5	DMS	C	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.42	0
5	DMS	C	8021	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
5	DMS	A	8003	-	3,3,3	2.60	1 (33%)	3,3,3	0.55	0
5	DMS	C	8025	-	3,3,3	2.59	1 (33%)	3,3,3	0.56	0
5	DMS	B	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
5	DMS	D	8017	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
5	DMS	B	8020	4	3,3,3	2.63	1 (33%)	3,3,3	0.50	0
5	DMS	C	8020	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
5	DMS	A	8019	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
5	DMS	B	8026	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
5	DMS	A	8013	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
5	DMS	C	8016	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
5	DMS	C	8012	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
5	DMS	A	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.43	0
5	DMS	B	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
5	DMS	B	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.56	0
5	DMS	D	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.43	0
5	DMS	D	8022	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
5	DMS	D	8023	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
5	DMS	B	8001	-	3,3,3	2.54	1 (33%)	3,3,3	0.37	0
5	DMS	B	8010	-	3,3,3	2.62	1 (33%)	3,3,3	0.41	0
5	DMS	D	8018	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
5	DMS	D	8008	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
5	DMS	B	8008	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
5	DMS	A	8018	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8007	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
5	DMS	B	8028	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
5	DMS	C	8003	-	3,3,3	2.59	1 (33%)	3,3,3	0.46	0
5	DMS	D	8003	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
5	DMS	B	8022	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
5	DMS	B	8005	-	3,3,3	2.66	1 (33%)	3,3,3	0.42	0
5	DMS	C	8006	-	3,3,3	2.62	1 (33%)	3,3,3	0.43	0
2	149	A	2001	4	12,12,12	2.58	2 (16%)	15,17,17	1.36	2 (13%)
5	DMS	A	8017	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
5	DMS	C	8017	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
5	DMS	B	8014	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
5	DMS	C	8014	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
5	DMS	D	8010	-	3,3,3	2.63	1 (33%)	3,3,3	0.43	0
5	DMS	A	8015	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
5	DMS	A	8023	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
5	DMS	A	8012	-	3,3,3	2.62	1 (33%)	3,3,3	0.45	0
5	DMS	B	8027	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
5	DMS	A	8028	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
5	DMS	C	8015	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
5	DMS	B	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
5	DMS	A	8024	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
5	DMS	C	8001	-	3,3,3	2.60	1 (33%)	3,3,3	0.53	0
5	DMS	A	8022	4	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
5	DMS	C	8022	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
5	DMS	B	8021	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
5	DMS	D	8025	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
5	DMS	D	8013	-	3,3,3	2.61	1 (33%)	3,3,3	0.44	0
5	DMS	D	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.37	0
5	DMS	A	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
2	149	B	2001	4	12,12,12	2.36	2 (16%)	15,17,17	1.06	2 (13%)
5	DMS	A	8027	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
5	DMS	B	8023	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
5	DMS	A	8029	-	3,3,3	2.59	1 (33%)	3,3,3	0.39	0
5	DMS	C	8018	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
5	DMS	D	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8003	-	3,3,3	2.59	1 (33%)	3,3,3	0.46	0
5	DMS	C	8011	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
5	DMS	A	8009	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
5	DMS	D	8001	-	3,3,3	2.54	1 (33%)	3,3,3	0.38	0
5	DMS	A	8008	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
5	DMS	D	8002	-	3,3,3	2.52	1 (33%)	3,3,3	0.56	0
5	DMS	D	8016	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
5	DMS	A	8010	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
5	DMS	A	8005	-	3,3,3	2.60	1 (33%)	3,3,3	0.43	0
2	149	C	2001	4	12,12,12	2.13	1 (8%)	15,17,17	1.19	2 (13%)
5	DMS	D	8006	-	3,3,3	2.62	1 (33%)	3,3,3	0.43	0
5	DMS	B	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.46	0
5	DMS	C	8024	-	3,3,3	2.68	1 (33%)	3,3,3	0.49	0
5	DMS	C	8023	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
5	DMS	D	8012	-	3,3,3	2.63	1 (33%)	3,3,3	0.52	0
5	DMS	A	8002	-	3,3,3	2.53	1 (33%)	3,3,3	0.40	0
5	DMS	D	8011	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
5	DMS	A	8004	-	3,3,3	2.60	1 (33%)	3,3,3	0.39	0
5	DMS	A	8026	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
5	DMS	C	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
5	DMS	A	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
5	DMS	A	8025	-	3,3,3	2.61	1 (33%)	3,3,3	0.51	0
5	DMS	D	8021	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
5	DMS	A	8006	-	3,3,3	2.64	1 (33%)	3,3,3	0.36	0
5	DMS	A	8016	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
5	DMS	A	8001	-	3,3,3	2.54	1 (33%)	3,3,3	0.52	0
5	DMS	D	8009	-	3,3,3	2.64	1 (33%)	3,3,3	0.41	0
5	DMS	B	8006	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
5	DMS	B	8012	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
5	DMS	D	8015	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
5	DMS	B	8011	-	3,3,3	2.60	1 (33%)	3,3,3	0.51	0
5	DMS	C	8013	-	3,3,3	2.60	1 (33%)	3,3,3	0.49	0
5	DMS	B	8025	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
5	DMS	B	8018	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
5	DMS	A	8011	-	3,3,3	2.61	1 (33%)	3,3,3	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	D	8024	-	3,3,3	2.65	1 (33%)	3,3,3	0.59	0
5	DMS	A	8021	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
5	DMS	C	8010	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
5	DMS	C	8009	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
5	DMS	C	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
5	DMS	D	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
5	DMS	D	8005	-	3,3,3	2.60	1 (33%)	3,3,3	0.54	0
5	DMS	B	8016	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	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
2	149	A	2001	4	-	1/2/22/22	0/1/1/1
2	149	B	2001	4	-	1/2/22/22	0/1/1/1
2	149	C	2001	4	-	1/2/22/22	0/1/1/1
2	149	D	2001	4	-	1/2/22/22	0/1/1/1

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	149	O5-C1	8.52	1.47	1.34
2	B	2001	149	O5-C1	7.78	1.46	1.34
2	D	2001	149	O5-C1	7.50	1.45	1.34
2	C	2001	149	O5-C1	7.16	1.45	1.34
5	B	8015	DMS	O-S	4.52	1.80	1.50
5	D	8016	DMS	O-S	4.51	1.80	1.50
5	A	8022	DMS	O-S	4.51	1.80	1.50
5	D	8023	DMS	O-S	4.50	1.80	1.50
5	C	8009	DMS	O-S	4.49	1.80	1.50
5	C	8024	DMS	O-S	4.49	1.80	1.50
5	B	8018	DMS	O-S	4.49	1.80	1.50
5	D	8025	DMS	O-S	4.49	1.80	1.50
5	A	8026	DMS	O-S	4.49	1.80	1.50
5	B	8014	DMS	O-S	4.49	1.80	1.50
5	A	8013	DMS	O-S	4.48	1.80	1.50
5	A	8017	DMS	O-S	4.48	1.80	1.50
5	B	8028	DMS	O-S	4.48	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8007	DMS	O-S	4.48	1.80	1.50
5	D	8018	DMS	O-S	4.48	1.80	1.50
5	B	8016	DMS	O-S	4.48	1.80	1.50
5	C	8016	DMS	O-S	4.48	1.80	1.50
5	C	8010	DMS	O-S	4.48	1.80	1.50
5	B	8026	DMS	O-S	4.48	1.80	1.50
5	C	8008	DMS	O-S	4.48	1.80	1.50
5	C	8023	DMS	O-S	4.48	1.80	1.50
5	B	8008	DMS	O-S	4.48	1.80	1.50
5	A	8007	DMS	O-S	4.48	1.80	1.50
5	B	8005	DMS	O-S	4.47	1.80	1.50
5	D	8017	DMS	O-S	4.47	1.80	1.50
5	A	8009	DMS	O-S	4.47	1.80	1.50
5	D	8024	DMS	O-S	4.47	1.80	1.50
5	C	8017	DMS	O-S	4.47	1.80	1.50
5	C	8018	DMS	O-S	4.46	1.80	1.50
5	A	8027	DMS	O-S	4.46	1.80	1.50
5	B	8022	DMS	O-S	4.46	1.80	1.50
5	A	8021	DMS	O-S	4.46	1.80	1.50
5	D	8015	DMS	O-S	4.46	1.80	1.50
5	A	8020	DMS	O-S	4.46	1.80	1.50
5	D	8019	DMS	O-S	4.46	1.80	1.50
5	A	8023	DMS	O-S	4.46	1.80	1.50
5	B	8019	DMS	O-S	4.46	1.80	1.50
5	A	8018	DMS	O-S	4.46	1.80	1.50
5	D	8021	DMS	O-S	4.46	1.80	1.50
5	B	8024	DMS	O-S	4.46	1.80	1.50
5	A	8014	DMS	O-S	4.46	1.80	1.50
5	D	8020	DMS	O-S	4.46	1.80	1.50
5	A	8006	DMS	O-S	4.46	1.80	1.50
5	C	8015	DMS	O-S	4.45	1.80	1.50
5	D	8014	DMS	O-S	4.45	1.80	1.50
5	A	8024	DMS	O-S	4.45	1.80	1.50
5	B	8023	DMS	O-S	4.45	1.80	1.50
5	B	8006	DMS	O-S	4.45	1.80	1.50
5	B	8027	DMS	O-S	4.45	1.80	1.50
5	D	8004	DMS	O-S	4.45	1.80	1.50
5	C	8020	DMS	O-S	4.45	1.80	1.50
5	B	8012	DMS	O-S	4.45	1.80	1.50
5	B	8017	DMS	O-S	4.45	1.80	1.50
5	B	8009	DMS	O-S	4.44	1.80	1.50
5	A	8019	DMS	O-S	4.44	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8004	DMS	O-S	4.44	1.80	1.50
5	A	8010	DMS	O-S	4.44	1.80	1.50
5	B	8013	DMS	O-S	4.44	1.80	1.50
5	B	8007	DMS	O-S	4.44	1.80	1.50
5	A	8016	DMS	O-S	4.44	1.80	1.50
5	B	8021	DMS	O-S	4.44	1.80	1.50
5	C	8022	DMS	O-S	4.44	1.80	1.50
5	C	8021	DMS	O-S	4.43	1.80	1.50
5	A	8015	DMS	O-S	4.43	1.80	1.50
5	D	8009	DMS	O-S	4.43	1.80	1.50
5	A	8008	DMS	O-S	4.42	1.80	1.50
5	C	8012	DMS	O-S	4.42	1.80	1.50
5	D	8008	DMS	O-S	4.42	1.80	1.50
5	C	8014	DMS	O-S	4.42	1.80	1.50
5	D	8007	DMS	O-S	4.42	1.80	1.50
5	B	8025	DMS	O-S	4.42	1.80	1.50
5	A	8028	DMS	O-S	4.41	1.80	1.50
5	D	8012	DMS	O-S	4.41	1.80	1.50
5	D	8003	DMS	O-S	4.41	1.80	1.50
5	D	8010	DMS	O-S	4.41	1.80	1.50
5	C	8019	DMS	O-S	4.40	1.80	1.50
5	C	8006	DMS	O-S	4.40	1.80	1.50
5	D	8006	DMS	O-S	4.40	1.80	1.50
5	B	8020	DMS	O-S	4.40	1.80	1.50
5	A	8012	DMS	O-S	4.39	1.79	1.50
5	B	8010	DMS	O-S	4.39	1.79	1.50
5	C	8004	DMS	O-S	4.38	1.79	1.50
5	A	8011	DMS	O-S	4.38	1.79	1.50
5	C	8011	DMS	O-S	4.38	1.79	1.50
5	C	8025	DMS	O-S	4.38	1.79	1.50
5	D	8022	DMS	O-S	4.38	1.79	1.50
5	D	8013	DMS	O-S	4.37	1.79	1.50
5	A	8004	DMS	O-S	4.37	1.79	1.50
5	B	8002	DMS	O-S	4.37	1.79	1.50
5	C	8001	DMS	O-S	4.36	1.79	1.50
5	A	8025	DMS	O-S	4.36	1.79	1.50
5	A	8003	DMS	O-S	4.36	1.79	1.50
5	A	8005	DMS	O-S	4.36	1.79	1.50
5	C	8003	DMS	O-S	4.36	1.79	1.50
5	B	8011	DMS	O-S	4.36	1.79	1.50
5	A	8029	DMS	O-S	4.36	1.79	1.50
5	C	8013	DMS	O-S	4.35	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8002	DMS	O-S	4.35	1.79	1.50
5	D	8005	DMS	O-S	4.35	1.79	1.50
5	C	8005	DMS	O-S	4.35	1.79	1.50
5	D	8011	DMS	O-S	4.34	1.79	1.50
5	B	8003	DMS	O-S	4.33	1.79	1.50
5	D	8001	DMS	O-S	4.27	1.79	1.50
5	A	8002	DMS	O-S	4.26	1.79	1.50
5	B	8001	DMS	O-S	4.26	1.79	1.50
5	A	8001	DMS	O-S	4.25	1.78	1.50
5	D	8002	DMS	O-S	4.23	1.78	1.50
2	D	2001	149	O5-C5	-2.26	1.43	1.46
2	A	2001	149	O5-C5	-2.08	1.43	1.46
2	B	2001	149	O5-C5	-2.07	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	149	O5-C1-C2	3.98	125.14	119.20
2	D	2001	149	O5-C1-C2	3.44	124.33	119.20
2	C	2001	149	O5-C1-C2	3.08	123.79	119.20
2	C	2001	149	O5-C5-C4	2.54	114.24	109.73
2	B	2001	149	O5-C1-C2	2.47	122.89	119.20
2	B	2001	149	O5-C5-C4	2.30	113.81	109.73
2	D	2001	149	O5-C5-C4	2.24	113.72	109.73
2	A	2001	149	O5-C1-O1	-2.04	115.49	118.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	149	O5-C5-C6-O6
2	D	2001	149	O5-C5-C6-O6
2	A	2001	149	O5-C5-C6-O6
2	C	2001	149	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8025	DMS	3	0
5	B	8028	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	149	1	0
5	D	8024	DMS	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	1015/1052 (96%)	0.04	27 (2%)	54	60	10, 19, 42, 71	0
1	B	1015/1052 (96%)	0.10	25 (2%)	57	63	12, 22, 39, 71	0
1	C	1015/1052 (96%)	0.15	35 (3%)	45	51	12, 21, 39, 75	0
1	D	1015/1052 (96%)	0.15	47 (4%)	32	38	10, 20, 41, 73	0
All	All	4060/4208 (96%)	0.11	134 (3%)	46	53	10, 20, 40, 75	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	730	LEU	9.9
1	A	733	ALA	8.0
1	C	735	HIS	6.3
1	A	730	LEU	5.7
1	D	686	PRO	5.6
1	A	11	LEU	5.4
1	C	731	PRO	4.9
1	C	685	LEU	4.8
1	C	689	GLU	4.7
1	A	685	LEU	4.5
1	A	801	ILE	4.4
1	C	801	ILE	4.4
1	D	831	ALA	4.4
1	A	735	HIS	4.3
1	C	745	MET	4.3
1	C	687	GLN	4.3
1	D	76	CYS	4.3
1	B	799	THR	4.3
1	B	12	GLN	4.2
1	B	9	VAL	4.2
1	B	731	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	10	VAL	4.1
1	D	734	SER	4.0
1	B	732	ALA	4.0
1	B	685	LEU	3.9
1	B	580	GLU	3.8
1	A	1022	GLN	3.8
1	D	799	THR	3.8
1	B	11	LEU	3.8
1	D	984	LEU	3.8
1	D	801	ILE	3.7
1	D	1023	LYS	3.6
1	A	1023	LYS	3.6
1	A	732	ALA	3.6
1	A	655	MET	3.6
1	D	772	ASP	3.5
1	C	9	VAL	3.5
1	D	860	GLY	3.5
1	A	580	GLU	3.5
1	A	737	ILE	3.5
1	C	12	GLN	3.5
1	B	686	PRO	3.4
1	D	753	ASN	3.4
1	C	730	LEU	3.4
1	A	12	GLN	3.3
1	A	686	PRO	3.3
1	D	858	ILE	3.3
1	C	682	LEU	3.2
1	A	9	VAL	3.2
1	C	11	LEU	3.2
1	B	801	ILE	3.1
1	C	732	ALA	3.1
1	B	689	GLU	3.1
1	D	685	LEU	3.1
1	B	263	GLY	3.1
1	B	730	LEU	3.1
1	D	733	ALA	3.1
1	D	735	HIS	3.0
1	D	10	VAL	3.0
1	A	689	GLU	3.0
1	C	736	ALA	3.0
1	C	690	SER	2.9
1	D	731	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	656	VAL	2.8
1	C	663	LEU	2.8
1	D	732	ALA	2.8
1	D	689	GLU	2.8
1	D	819	GLU	2.8
1	A	663	LEU	2.8
1	D	846	GLY	2.8
1	D	11	LEU	2.7
1	D	687	GLN	2.7
1	A	76	CYS	2.7
1	D	737	ILE	2.7
1	D	9	VAL	2.7
1	D	827	ALA	2.6
1	D	861	SER	2.6
1	C	831	ALA	2.6
1	B	79	PRO	2.6
1	A	682	LEU	2.6
1	C	772	ASP	2.5
1	D	770	ILE	2.5
1	C	478	VAL	2.5
1	B	95	TYR	2.5
1	C	845	GLN	2.5
1	A	10	VAL	2.4
1	B	687	GLN	2.4
1	B	76	CYS	2.4
1	C	76	CYS	2.4
1	D	745	MET	2.4
1	C	728	VAL	2.4
1	C	684	GLU	2.4
1	B	1022	GLN	2.4
1	C	737	ILE	2.4
1	C	734	SER	2.4
1	A	731	PRO	2.3
1	B	819	GLU	2.3
1	C	832	ASP	2.3
1	B	69	VAL	2.3
1	D	728	VAL	2.3
1	C	251	ARG	2.3
1	D	889	ALA	2.3
1	D	948	PRO	2.3
1	C	634	GLN	2.2
1	C	891	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	820	ALA	2.2
1	D	1022	GLN	2.2
1	D	829	THR	2.2
1	C	733	ALA	2.2
1	B	663	LEU	2.2
1	D	832	ASP	2.2
1	C	758	PHE	2.2
1	D	866	ILE	2.2
1	D	752	GLY	2.2
1	D	179	ALA	2.2
1	D	736	ALA	2.2
1	A	861	SER	2.1
1	A	728	VAL	2.1
1	A	751	LEU	2.1
1	D	836	ILE	2.1
1	B	74	LEU	2.1
1	A	749	ILE	2.1
1	A	768	MET	2.1
1	B	800	ARG	2.1
1	A	687	GLN	2.1
1	D	768	MET	2.1
1	D	841	ALA	2.1
1	D	751	LEU	2.1
1	B	737	ILE	2.1
1	B	761	GLN	2.0
1	C	651	LEU	2.0
1	D	691	ALA	2.0
1	D	690	SER	2.0
1	C	74	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, 95^{th} 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	A	8013	4/4	0.58	0.38	100,100,101,101	0
5	DMS	B	8015	4/4	0.62	0.25	54,55,57,60	0
5	DMS	B	8026	4/4	0.67	0.24	78,78,78,80	0
5	DMS	B	8006	4/4	0.73	0.32	56,59,60,62	0
5	DMS	C	8016	4/4	0.77	0.18	54,58,59,63	0
5	DMS	A	8007	4/4	0.77	0.21	43,49,52,54	0
5	DMS	C	8023	4/4	0.78	0.34	53,54,56,57	0
5	DMS	B	8013	4/4	0.79	0.25	31,32,35,44	0
5	DMS	B	8007	4/4	0.79	0.51	94,94,95,95	0
5	DMS	D	8007	4/4	0.79	0.26	52,52,53,56	0
5	DMS	B	8022	4/4	0.80	0.22	54,54,54,56	0
5	DMS	D	8016	4/4	0.81	0.19	38,40,45,53	0
5	DMS	C	8007	4/4	0.81	0.16	53,56,56,57	0
5	DMS	D	8022	4/4	0.82	0.15	21,29,33,45	0
5	DMS	A	8027	4/4	0.82	0.24	48,48,52,53	0
5	DMS	A	8017	4/4	0.82	0.18	43,43,47,54	0
5	DMS	C	8024	4/4	0.83	0.21	51,53,53,54	0
5	DMS	B	8016	4/4	0.83	0.18	55,55,57,60	0
5	DMS	D	8017	4/4	0.84	0.32	71,73,74,74	0
5	DMS	C	8019	4/4	0.85	0.26	36,36,38,39	4
5	DMS	A	8019	4/4	0.85	0.18	61,61,61,62	0
5	DMS	D	8010	4/4	0.86	0.28	41,46,48,50	0
5	DMS	A	8018	4/4	0.86	0.18	71,72,72,74	0
5	DMS	C	8010	4/4	0.86	0.30	61,63,63,64	0
5	DMS	B	8009	4/4	0.86	0.20	51,54,55,55	0
5	DMS	C	8004	4/4	0.86	0.14	27,29,35,37	0
5	DMS	A	8023	4/4	0.87	0.17	50,52,54,55	0
5	DMS	C	8015	4/4	0.87	0.20	47,49,52,53	0
5	DMS	D	8019	4/4	0.87	0.23	59,59,60,61	0
5	DMS	D	8023	4/4	0.88	0.16	38,39,40,44	0
5	DMS	B	8023	4/4	0.88	0.22	45,47,49,51	0
5	DMS	C	8018	4/4	0.88	0.15	55,57,57,59	0
5	DMS	C	8013	4/4	0.88	0.20	30,36,39,43	0
5	DMS	A	8024	4/4	0.89	0.12	30,34,40,42	0
5	DMS	A	8016	4/4	0.89	0.12	44,47,47,50	0
5	DMS	B	8014	4/4	0.89	0.23	58,60,60,60	0
5	DMS	B	8020	4/4	0.89	0.56	50,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8008	4/4	0.90	0.12	43,46,47,51	0
5	DMS	A	8022	4/4	0.90	0.17	37,44,44,48	0
5	DMS	B	8018	4/4	0.90	0.12	54,55,55,55	0
4	NA	D	3104	1/1	0.90	0.15	41,41,41,41	0
5	DMS	D	8021	4/4	0.90	0.23	49,50,51,52	0
5	DMS	A	8006	4/4	0.90	0.17	30,33,41,42	0
5	DMS	D	8020	4/4	0.90	0.28	53,54,57,57	0
5	DMS	A	8015	4/4	0.91	0.19	39,43,46,48	0
5	DMS	B	8004	4/4	0.91	0.12	39,44,44,44	0
5	DMS	C	8022	4/4	0.91	0.21	47,48,50,51	0
5	DMS	D	8015	4/4	0.91	0.11	43,44,44,51	0
3	MG	B	3003	1/1	0.91	0.18	27,27,27,27	1
5	DMS	B	8025	4/4	0.92	0.26	49,53,54,56	0
5	DMS	A	8004	4/4	0.92	0.10	34,34,40,42	0
5	DMS	C	8014	4/4	0.92	0.19	36,37,40,41	0
4	NA	A	3104	1/1	0.92	0.15	32,32,32,32	0
5	DMS	B	8012	4/4	0.92	0.16	40,45,45,50	0
5	DMS	D	8006	4/4	0.92	0.14	42,43,44,47	0
5	DMS	D	8004	4/4	0.92	0.20	41,46,47,49	0
5	DMS	B	8017	4/4	0.92	0.14	41,44,47,47	0
5	DMS	A	8014	4/4	0.93	0.17	45,48,50,52	0
5	DMS	D	8018	4/4	0.93	0.12	53,54,54,55	0
5	DMS	B	8011	4/4	0.93	0.14	31,34,37,39	0
5	DMS	D	8008	4/4	0.93	0.14	29,33,34,38	0
5	DMS	C	8020	4/4	0.93	0.10	59,59,61,61	0
4	NA	C	3104	1/1	0.93	0.23	37,37,37,37	0
3	MG	A	3002	1/1	0.94	0.08	17,17,17,17	0
5	DMS	B	8024	4/4	0.94	0.14	52,54,55,60	0
5	DMS	C	8006	4/4	0.94	0.22	71,71,71,72	0
5	DMS	A	8021	4/4	0.94	0.14	55,55,55,57	0
2	149	A	2001	12/12	0.94	0.09	12,14,17,21	0
5	DMS	C	8021	4/4	0.94	0.08	37,40,43,44	0
5	DMS	B	8021	4/4	0.94	0.16	49,52,52,53	0
5	DMS	B	8019	4/4	0.94	0.10	48,48,49,51	0
5	DMS	D	8011	4/4	0.94	0.11	27,30,31,31	0
5	DMS	C	8017	4/4	0.94	0.14	53,53,56,56	0
5	DMS	B	8027	4/4	0.95	0.10	47,49,50,52	0
5	DMS	C	8012	4/4	0.95	0.12	36,37,38,40	0
5	DMS	A	8008	4/4	0.95	0.20	37,38,41,42	0
3	MG	A	3005	1/1	0.95	0.10	39,39,39,39	0
5	DMS	A	8028	4/4	0.95	0.22	43,46,47,48	0
5	DMS	B	8008	4/4	0.95	0.12	31,32,34,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	B	3104	1/1	0.95	0.10	36,36,36,36	0
5	DMS	A	8020	4/4	0.95	0.11	41,46,46,48	0
5	DMS	C	8011	4/4	0.95	0.13	29,32,33,37	0
5	DMS	A	8012	4/4	0.95	0.18	31,32,37,38	0
3	MG	C	3002	1/1	0.95	0.12	16,16,16,16	0
4	NA	C	3103	1/1	0.96	0.07	31,31,31,31	0
5	DMS	A	8025	4/4	0.96	0.13	26,30,37,38	0
2	149	D	2001	12/12	0.96	0.07	11,13,14,21	0
5	DMS	B	8003	4/4	0.96	0.11	25,26,29,29	0
5	DMS	A	8009	4/4	0.96	0.09	35,37,37,40	0
5	DMS	D	8009	4/4	0.96	0.10	34,35,37,37	0
5	DMS	C	8005	4/4	0.96	0.15	31,35,35,38	0
4	NA	C	3102	1/1	0.96	0.06	17,17,17,17	0
5	DMS	B	8028	4/4	0.96	0.14	26,29,32,36	0
5	DMS	C	8003	4/4	0.96	0.10	28,28,29,33	0
5	DMS	D	8013	4/4	0.96	0.16	28,37,39,40	0
4	NA	A	3103	1/1	0.96	0.08	27,27,27,27	0
5	DMS	A	8010	4/4	0.96	0.20	58,58,58,59	0
2	149	C	2001	12/12	0.96	0.09	7,12,14,25	0
5	DMS	B	8005	4/4	0.96	0.13	35,36,37,38	0
2	149	B	2001	12/12	0.96	0.08	13,14,19,26	0
5	DMS	D	8012	4/4	0.96	0.13	31,35,36,39	0
5	DMS	C	8009	4/4	0.96	0.16	39,40,41,42	0
5	DMS	C	8025	4/4	0.96	0.16	34,36,40,40	0
5	DMS	D	8014	4/4	0.96	0.15	28,30,37,39	0
5	DMS	A	8026	4/4	0.96	0.14	40,41,42,42	0
5	DMS	A	8029	4/4	0.96	0.10	28,31,32,33	0
5	DMS	C	8002	4/4	0.97	0.08	22,24,25,26	0
4	NA	D	3103	1/1	0.97	0.07	33,33,33,33	0
5	DMS	A	8003	4/4	0.97	0.10	20,23,24,26	0
5	DMS	A	8011	4/4	0.97	0.09	29,32,32,32	0
5	DMS	D	8024	4/4	0.97	0.09	26,26,33,33	0
5	DMS	D	8025	4/4	0.97	0.09	30,31,32,33	0
5	DMS	D	8002	4/4	0.97	0.11	19,21,22,24	0
5	DMS	B	8002	4/4	0.97	0.11	23,25,29,31	0
5	DMS	B	8001	4/4	0.97	0.10	17,19,19,26	0
4	NA	B	3102	1/1	0.97	0.07	17,17,17,17	0
5	DMS	B	8010	4/4	0.97	0.15	34,39,40,46	0
3	MG	A	3003	1/1	0.97	0.08	31,31,31,31	0
3	MG	B	3002	1/1	0.97	0.08	21,21,21,21	0
5	DMS	C	8001	4/4	0.97	0.06	18,20,25,26	0
3	MG	D	3001	1/1	0.98	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	D	8001	4/4	0.98	0.08	16,17,21,21	0
3	MG	D	3002	1/1	0.98	0.04	16,16,16,16	0
4	NA	D	3101	1/1	0.98	0.07	15,15,15,15	0
5	DMS	A	8001	4/4	0.98	0.07	15,20,21,22	0
5	DMS	D	8005	4/4	0.98	0.10	24,28,28,29	0
5	DMS	A	8002	4/4	0.98	0.10	20,22,24,24	0
4	NA	A	3101	1/1	0.99	0.05	12,12,12,12	0
3	MG	B	3001	1/1	0.99	0.04	18,18,18,18	0
5	DMS	D	8003	4/4	0.99	0.09	24,25,26,28	0
4	NA	C	3101	1/1	0.99	0.05	17,17,17,17	0
4	NA	B	3103	1/1	0.99	0.06	25,25,25,25	0
4	NA	A	3102	1/1	0.99	0.06	17,17,17,17	0
4	NA	D	3102	1/1	0.99	0.05	16,16,16,16	0
5	DMS	A	8005	4/4	0.99	0.08	25,26,28,31	0
4	NA	B	3101	1/1	0.99	0.05	15,15,15,15	0
3	MG	A	3001	1/1	0.99	0.06	12,12,12,12	0
3	MG	C	3001	1/1	1.00	0.09	11,11,11,11	0

6.5 Other polymers

There are no such residues in this entry.