Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 02:26 PM EST

PDB ID	:	3T0A
Title	:	E. coli (LacZ) beta-galactosidase (S796T)
Authors	:	Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.
Deposited on	:	2011-07-19
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

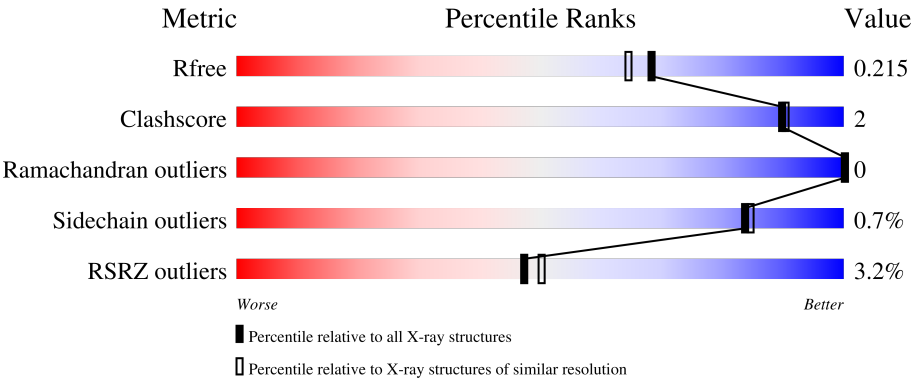
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	B	8013	-	-	-	X
4	DMS	D	8010	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 36814 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
			8158	5160	1445	1515	38			
1	B	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			
1	C	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			
1	D	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	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	THR	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	THR	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	THR	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	THR	SER	engineered mutation	UNP P00722

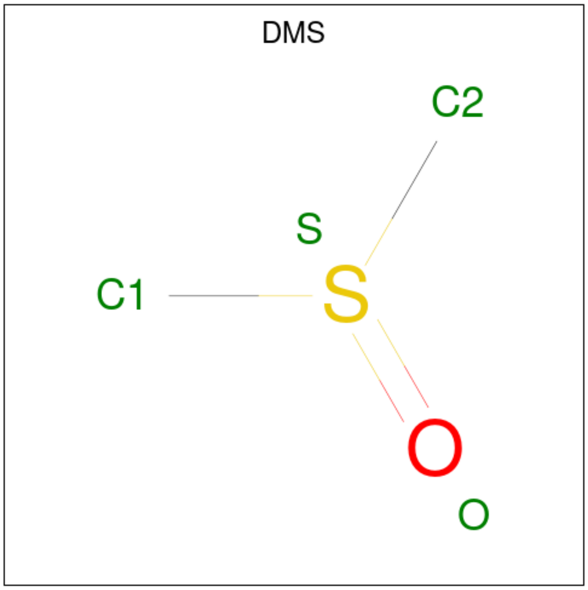
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

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

- Molecule 5 is water.

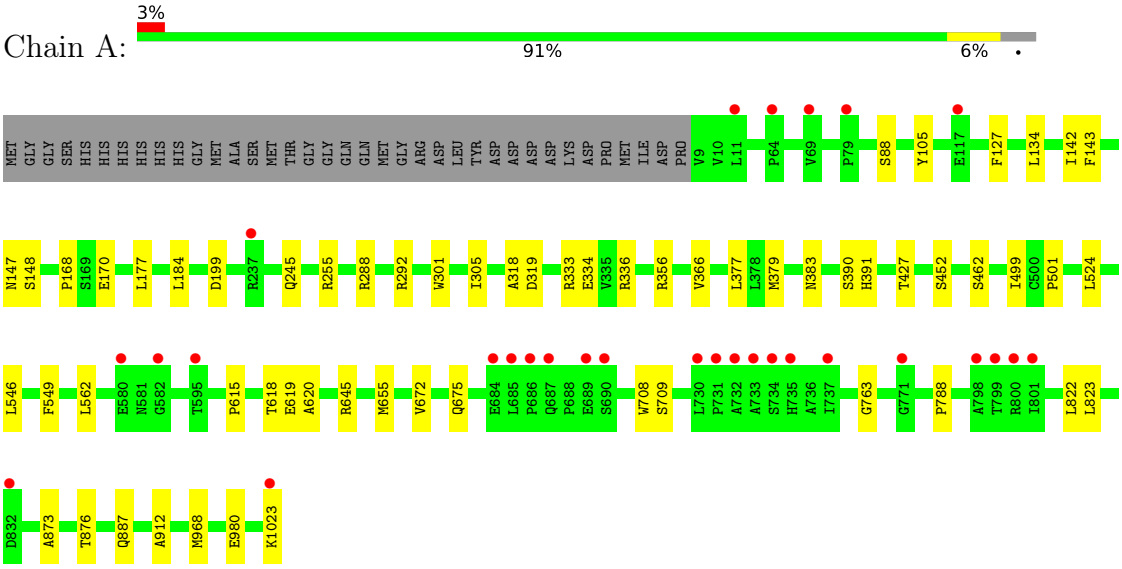
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	850	Total O 850 850	0	0
5	B	979	Total O 979 979	0	0
5	C	1009	Total O 1009 1009	0	0
5	D	875	Total O 875 875	0	0

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.

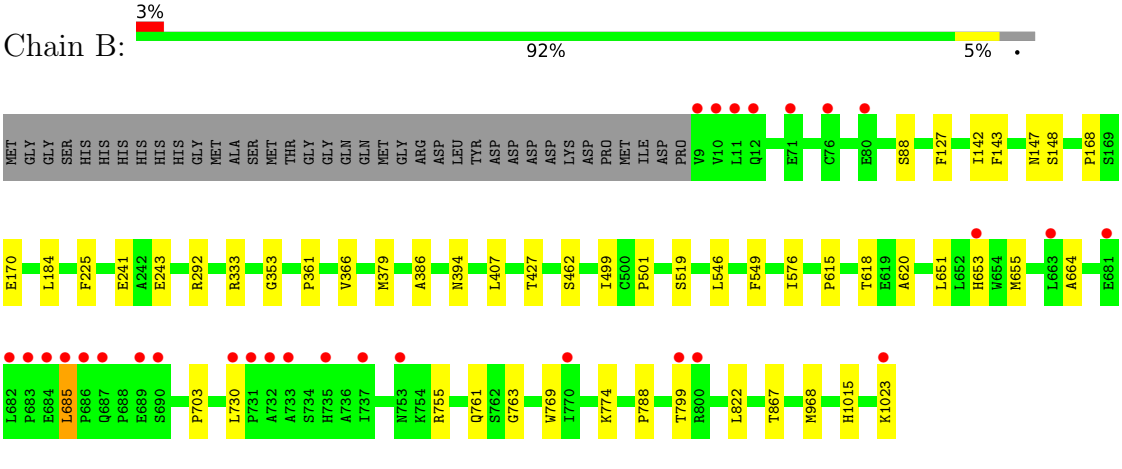
• Molecule 1: Beta-galactosidase

Chain A:



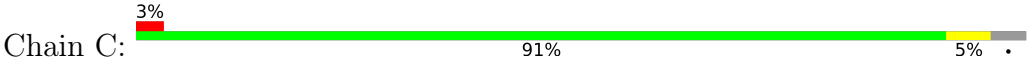
• Molecule 1: Beta-galactosidase

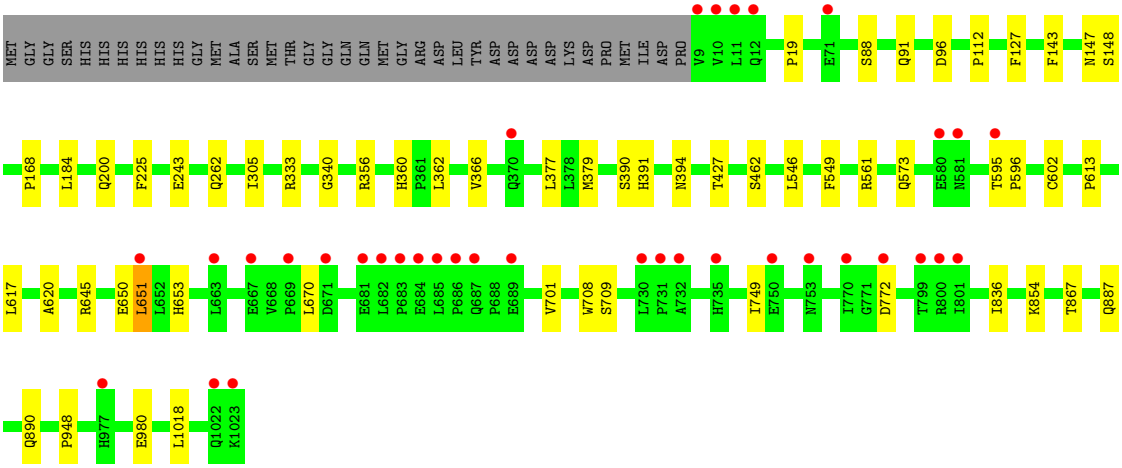
Chain B:



• Molecule 1: Beta-galactosidase

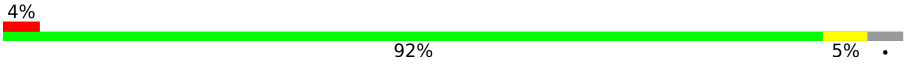
Chain C:

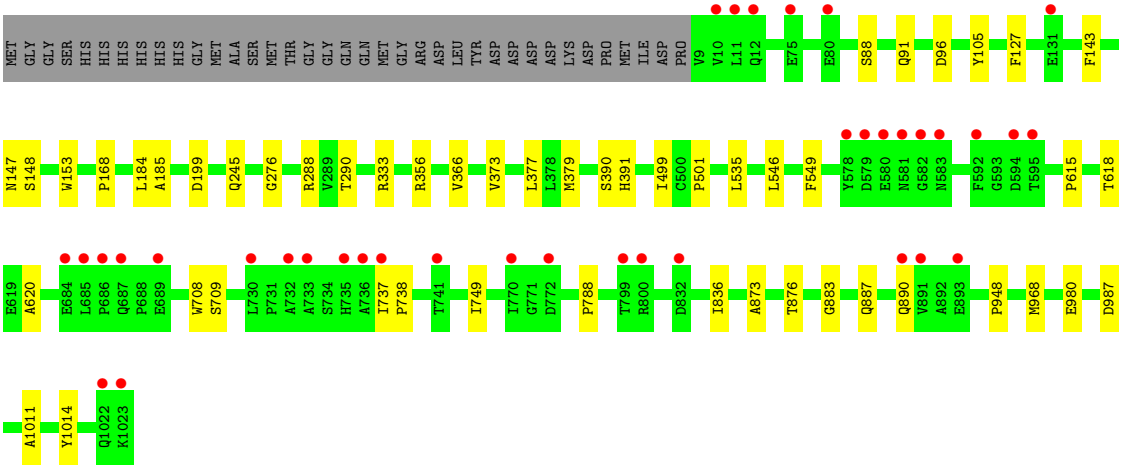




• Molecule 1: Beta-galactosidase

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	150.92Å 161.22Å 202.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.72 – 1.90 56.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.72-1.90) 92.7 (56.68-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.170 , 0.214 0.172 , 0.215	Depositor DCC
R_{free} test set	5178 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36814	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 40.74 % 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 2.6181e-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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	0/8400	0.52	0/11460
1	B	0.37	0/8400	0.53	0/11460
1	C	0.37	0/8400	0.53	1/11460 (0.0%)
1	D	0.35	0/8400	0.52	0/11460
All	All	0.36	0/33600	0.52	1/45840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1018	LEU	CA-CB-CG	5.29	127.46	115.30

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	8158	0	7755	32	0
1	B	8158	0	7755	25	0
1	C	8158	0	7755	28	0
1	D	8158	0	7755	31	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	5	0	0	0	0
4	A	92	0	138	3	0
4	B	128	0	192	0	0
4	C	128	0	192	0	0
4	D	92	0	138	4	0
5	A	850	0	0	2	0
5	B	979	0	0	0	0
5	C	1009	0	0	0	0
5	D	875	0	0	0	0
All	All	36814	0	31680	116	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 (116) 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:D:788:PRO:HD2	1:D:968:MET:HG3	1.75	0.68
1:A:887:GLN:NE2	1:A:980:GLU:O	2.30	0.62
4:A:8022:DMS:H23	5:A:4565:HOH:O	1.99	0.62
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.80	0.61
1:B:664:ALA:HB3	1:B:685:LEU:HD21	1.83	0.60
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.84	0.59
1:D:887:GLN:NE2	1:D:980:GLU:O	2.34	0.59
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.85	0.59
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.85	0.58
1:B:755:ARG:HB2	1:B:769:TRP:HB2	1.86	0.57
1:B:615:PRO:O	1:B:618:THR:HG22	2.05	0.57
1:B:241:GLU:HG2	1:B:292:ARG:HG2	1.87	0.57
1:D:615:PRO:O	1:D:618:THR:HG22	2.05	0.56
1:B:651:LEU:HD23	1:B:703:PRO:HG3	1.87	0.56
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.86	0.56
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.88	0.56
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.43	0.54
1:A:383:ASN:HA	4:A:8003:DMS:H21	1.89	0.54
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.08	0.53
1:D:356:ARG:HD2	1:D:379:MET:CE	2.39	0.53
1:A:88:SER:HA	1:A:366:VAL:HG21	1.92	0.52
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.45	0.51
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.93	0.51
1:D:88:SER:HA	1:D:366:VAL:HG21	1.93	0.51
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.73	0.50
1:B:788:PRO:HD2	1:B:968:MET:HG3	1.94	0.50
1:D:276:GLY:HA2	4:D:8010:DMS:H22	1.94	0.49
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.46	0.49
1:C:887:GLN:NE2	1:C:980:GLU:O	2.43	0.49
1:C:356:ARG:HD2	1:C:379:MET:CE	2.43	0.48
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.42	0.48
1:B:88:SER:HA	1:B:366:VAL:HG21	1.96	0.48
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.96	0.48
1:A:615:PRO:O	1:A:618:THR:HG22	2.14	0.48
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.95	0.48
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:D:356:ARG:HD2	1:D:379:MET:HE1	1.97	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.47
1:C:651:LEU:HD13	1:C:653:HIS:CD2	2.50	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.96	0.47
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.50	0.47
1:A:873:ALA:O	1:A:876:THR:HG22	2.15	0.47
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.97	0.46
1:D:276:GLY:HA2	4:D:8010:DMS:C2	2.45	0.46
1:C:360:HIS:HE1	1:C:362:LEU:HD12	1.79	0.46
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.52	0.45
1:A:292:ARG:HH12	4:A:8011:DMS:C1	2.29	0.45
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.99	0.45
1:A:427:THR:HG21	1:A:462:SER:HB3	1.98	0.45
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.52	0.45
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.81	0.45
1:A:390:SER:HA	1:A:391:HIS:HA	1.85	0.45
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.98	0.45
1:D:290:THR:H	4:D:8010:DMS:C2	2.30	0.45
1:C:854:LYS:HA	1:C:867:THR:O	2.17	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.63	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.52	0.44
1:A:823:LEU:O	1:B:730:LEU:HD11	2.17	0.44
1:B:769:TRP:NE1	1:B:774:LYS:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:PHE:O	1:C:168:PRO:HA	2.18	0.44
1:D:390:SER:HA	1:D:391:HIS:HA	1.82	0.44
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.61	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.62	0.43
1:B:143:PHE:O	1:B:168:PRO:HA	2.18	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.43
1:B:867:THR:HG23	1:B:1015:HIS:HE1	1.83	0.43
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.53	0.43
1:A:675:GLN:HG3	5:A:4412:HOH:O	2.19	0.43
1:C:88:SER:HA	1:C:366:VAL:HG21	1.99	0.43
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.43
1:C:650:GLU:HB3	1:C:670:LEU:HD12	2.01	0.43
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.54	0.43
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.99	0.42
1:B:361:PRO:HB2	1:B:576:ILE:HG12	1.99	0.42
1:C:19:PRO:HD3	1:C:112:PRO:CB	2.49	0.42
1:C:390:SER:HA	1:C:391:HIS:HA	1.79	0.42
1:C:651:LEU:HD12	1:C:701:VAL:HB	2.02	0.42
1:B:867:THR:HG23	1:B:1015:HIS:CE1	2.54	0.42
1:A:356:ARG:HD2	1:A:379:MET:CE	2.49	0.42
1:A:356:ARG:HD2	1:A:379:MET:HE1	2.01	0.42
1:B:427:THR:HG21	1:B:462:SER:HB3	2.02	0.42
1:C:595:THR:HA	1:C:596:PRO:C	2.40	0.42
1:D:153:TRP:HB2	1:D:185:ALA:HB3	2.02	0.42
1:A:143:PHE:O	1:A:168:PRO:HA	2.20	0.41
1:A:524:LEU:HD11	1:A:562:LEU:HG	2.02	0.41
1:A:134:LEU:HD21	1:A:177:LEU:HB2	2.03	0.41
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.41
1:C:427:THR:HG21	1:C:462:SER:HB3	2.02	0.41
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.19	0.41
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.84	0.41
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.95	0.41
1:D:890:GLN:OE1	1:D:948:PRO:HD3	2.19	0.41
1:C:749:ILE:HD11	1:C:836:ILE:HD11	2.02	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.56	0.41
1:D:290:THR:H	4:D:8010:DMS:H21	1.85	0.41
1:D:873:ALA:O	1:D:876:THR:HG22	2.20	0.41
1:B:379:MET:HE1	1:B:407:LEU:HD13	2.02	0.41
1:D:356:ARG:HD2	1:D:379:MET:HE3	2.03	0.41
1:D:373:VAL:O	1:D:377:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.56	0.41
1:A:255:ARG:HG3	1:A:318:ALA:HA	2.03	0.41
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.01	0.41
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.56	0.41
1:B:225:PHE:HA	1:B:243:GLU:O	2.21	0.41
1:C:340:GLY:O	1:C:561:ARG:HG2	2.21	0.41
1:A:301:TRP:CH2	1:A:452:SER:HA	2.56	0.40
1:D:749:ILE:HD11	1:D:836:ILE:HD11	2.03	0.40
1:C:225:PHE:HA	1:C:243:GLU:O	2.21	0.40
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.56	0.40
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.21	0.40
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.03	0.40
1:B:353:GLY:HA2	1:B:386:ALA:O	2.21	0.40
1:C:305:ILE:HD11	1:C:645:ARG:HB3	2.03	0.40
1:B:651:LEU:HD11	1:B:653:HIS:NE2	2.37	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%)	985 (97%)	28 (3%)	0	100	100
1	C	1013/1052 (96%)	983 (97%)	30 (3%)	0	100	100
1	D	1013/1052 (96%)	983 (97%)	30 (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	868/898 (97%)	862 (99%)	6 (1%)	84 84
1	B	868/898 (97%)	859 (99%)	9 (1%)	76 76
1	C	868/898 (97%)	862 (99%)	6 (1%)	84 84
1	D	868/898 (97%)	865 (100%)	3 (0%)	92 93
All	All	3472/3592 (97%)	3448 (99%)	24 (1%)	84 84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ASP
1	A	333	ARG
1	A	546	LEU
1	A	655	MET
1	A	672	VAL
1	A	1023	LYS
1	B	333	ARG
1	B	394	ASN
1	B	519	SER
1	B	546	LEU
1	B	655	MET
1	B	685	LEU
1	B	761	GLN
1	B	799	THR
1	B	1023	LYS
1	C	262	GLN
1	C	333	ARG
1	C	394	ASN
1	C	546	LEU
1	C	651	LEU
1	C	772	ASP
1	D	333	ARG
1	D	535	LEU
1	D	546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 139 ligands modelled in this entry, 29 are monoatomic - leaving 110 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	B	8013	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
4	DMS	B	8027	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
4	DMS	A	8015	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
4	DMS	A	8021	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
4	DMS	B	8017	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
4	DMS	C	8024	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
4	DMS	B	8015	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
4	DMS	C	8013	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	D	8003	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
4	DMS	D	8011	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
4	DMS	A	8020	-	3,3,3	2.65	1 (33%)	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	B	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
4	DMS	A	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
4	DMS	B	8018	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
4	DMS	D	8013	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	D	8016	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
4	DMS	C	8009	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0
4	DMS	C	8003	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
4	DMS	B	8022	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
4	DMS	B	8005	-	3,3,3	2.60	1 (33%)	3,3,3	0.31	0
4	DMS	C	8015	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
4	DMS	C	8012	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
4	DMS	B	8014	-	3,3,3	2.62	1 (33%)	3,3,3	0.47	0
4	DMS	A	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.50	0
4	DMS	A	8009	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
4	DMS	B	8003	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
4	DMS	D	8012	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	B	8007	-	3,3,3	2.65	1 (33%)	3,3,3	0.44	0
4	DMS	D	8009	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
4	DMS	D	8017	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
4	DMS	A	8004	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
4	DMS	C	8016	3	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
4	DMS	B	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
4	DMS	D	8020	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
4	DMS	B	8012	-	3,3,3	2.62	1 (33%)	3,3,3	0.43	0
4	DMS	A	8012	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
4	DMS	C	8028	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
4	DMS	B	8024	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
4	DMS	D	8002	-	3,3,3	2.58	1 (33%)	3,3,3	0.45	0
4	DMS	C	8023	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
4	DMS	A	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.41	0
4	DMS	D	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.39	0
4	DMS	C	8011	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
4	DMS	A	8022	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
4	DMS	B	8008	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
4	DMS	C	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	B	8009	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
4	DMS	D	8014	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
4	DMS	A	8001	-	3,3,3	2.58	1 (33%)	3,3,3	0.50	0
4	DMS	D	8001	-	3,3,3	2.59	1 (33%)	3,3,3	0.40	0
4	DMS	C	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
4	DMS	D	8015	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
4	DMS	B	8023	-	3,3,3	2.62	1 (33%)	3,3,3	0.45	0
4	DMS	D	8018	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	C	8018	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
4	DMS	D	8021	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
4	DMS	A	8003	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0
4	DMS	B	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
4	DMS	D	8004	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
4	DMS	B	8028	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
4	DMS	B	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.42	0
4	DMS	B	8021	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
4	DMS	D	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
4	DMS	A	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
4	DMS	C	8005	-	3,3,3	2.61	1 (33%)	3,3,3	0.37	0
4	DMS	C	8032	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
4	DMS	C	8026	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
4	DMS	C	8002	-	3,3,3	2.57	1 (33%)	3,3,3	0.53	0
4	DMS	A	8018	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
4	DMS	B	8004	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
4	DMS	C	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
4	DMS	B	8030	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
4	DMS	A	8008	-	3,3,3	2.68	1 (33%)	3,3,3	0.49	0
4	DMS	D	8008	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	A	8019	-	3,3,3	2.64	1 (33%)	3,3,3	0.45	0
4	DMS	D	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	C	8022	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
4	DMS	C	8031	-	3,3,3	2.60	1 (33%)	3,3,3	0.45	0
4	DMS	C	8030	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
4	DMS	B	8026	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
4	DMS	B	8002	-	3,3,3	2.53	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	A	8023	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
4	DMS	D	8023	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
4	DMS	A	8016	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
4	DMS	A	8006	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
4	DMS	C	8025	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
4	DMS	C	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
4	DMS	B	8019	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
4	DMS	C	8027	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
4	DMS	C	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
4	DMS	C	8008	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
4	DMS	A	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
4	DMS	C	8010	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
4	DMS	D	8022	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	C	8029	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
4	DMS	B	8025	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
4	DMS	B	8031	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
4	DMS	A	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	B	8029	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
4	DMS	B	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	C	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
4	DMS	B	8016	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
4	DMS	D	8006	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
4	DMS	A	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.45	0
4	DMS	C	8021	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	C	8004	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
4	DMS	D	8010	-	3,3,3	2.64	1 (33%)	3,3,3	0.37	0
4	DMS	C	8006	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
4	DMS	A	8014	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
4	DMS	B	8032	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8008	DMS	O-S	4.54	1.80	1.50
4	B	8009	DMS	O-S	4.54	1.80	1.50
4	A	8008	DMS	O-S	4.51	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8017	DMS	O-S	4.50	1.80	1.50
4	C	8006	DMS	O-S	4.50	1.80	1.50
4	D	8015	DMS	O-S	4.50	1.80	1.50
4	D	8014	DMS	O-S	4.49	1.80	1.50
4	B	8013	DMS	O-S	4.49	1.80	1.50
4	B	8021	DMS	O-S	4.49	1.80	1.50
4	C	8007	DMS	O-S	4.49	1.80	1.50
4	D	8007	DMS	O-S	4.49	1.80	1.50
4	C	8015	DMS	O-S	4.49	1.80	1.50
4	A	8015	DMS	O-S	4.48	1.80	1.50
4	A	8021	DMS	O-S	4.48	1.80	1.50
4	B	8022	DMS	O-S	4.48	1.80	1.50
4	A	8014	DMS	O-S	4.48	1.80	1.50
4	B	8016	DMS	O-S	4.48	1.80	1.50
4	B	8032	DMS	O-S	4.48	1.80	1.50
4	C	8028	DMS	O-S	4.48	1.80	1.50
4	C	8026	DMS	O-S	4.47	1.80	1.50
4	C	8020	DMS	O-S	4.47	1.80	1.50
4	A	8023	DMS	O-S	4.47	1.80	1.50
4	A	8007	DMS	O-S	4.47	1.80	1.50
4	B	8027	DMS	O-S	4.47	1.80	1.50
4	A	8004	DMS	O-S	4.47	1.80	1.50
4	C	8019	DMS	O-S	4.47	1.80	1.50
4	D	8016	DMS	O-S	4.47	1.80	1.50
4	C	8017	DMS	O-S	4.47	1.80	1.50
4	C	8021	DMS	O-S	4.47	1.80	1.50
4	D	8019	DMS	O-S	4.47	1.80	1.50
4	C	8012	DMS	O-S	4.46	1.80	1.50
4	C	8004	DMS	O-S	4.46	1.80	1.50
4	B	8006	DMS	O-S	4.46	1.80	1.50
4	D	8022	DMS	O-S	4.46	1.80	1.50
4	C	8013	DMS	O-S	4.46	1.80	1.50
4	B	8020	DMS	O-S	4.46	1.80	1.50
4	B	8029	DMS	O-S	4.46	1.80	1.50
4	D	8013	DMS	O-S	4.46	1.80	1.50
4	A	8022	DMS	O-S	4.46	1.80	1.50
4	D	8006	DMS	O-S	4.46	1.80	1.50
4	B	8015	DMS	O-S	4.46	1.80	1.50
4	D	8004	DMS	O-S	4.46	1.80	1.50
4	C	8029	DMS	O-S	4.46	1.80	1.50
4	C	8011	DMS	O-S	4.46	1.80	1.50
4	D	8010	DMS	O-S	4.46	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8016	DMS	O-S	4.45	1.80	1.50
4	A	8006	DMS	O-S	4.45	1.80	1.50
4	D	8023	DMS	O-S	4.45	1.80	1.50
4	D	8021	DMS	O-S	4.45	1.80	1.50
4	C	8018	DMS	O-S	4.45	1.80	1.50
4	A	8013	DMS	O-S	4.45	1.80	1.50
4	C	8014	DMS	O-S	4.45	1.80	1.50
4	B	8018	DMS	O-S	4.45	1.80	1.50
4	B	8004	DMS	O-S	4.45	1.80	1.50
4	B	8010	DMS	O-S	4.45	1.80	1.50
4	B	8028	DMS	O-S	4.45	1.80	1.50
4	A	8009	DMS	O-S	4.45	1.80	1.50
4	D	8008	DMS	O-S	4.45	1.80	1.50
4	B	8031	DMS	O-S	4.45	1.80	1.50
4	B	8030	DMS	O-S	4.45	1.80	1.50
4	A	8017	DMS	O-S	4.45	1.80	1.50
4	B	8007	DMS	O-S	4.45	1.80	1.50
4	C	8010	DMS	O-S	4.45	1.80	1.50
4	C	8030	DMS	O-S	4.45	1.80	1.50
4	C	8027	DMS	O-S	4.45	1.80	1.50
4	A	8019	DMS	O-S	4.44	1.80	1.50
4	B	8019	DMS	O-S	4.44	1.80	1.50
4	C	8022	DMS	O-S	4.44	1.80	1.50
4	B	8003	DMS	O-S	4.44	1.80	1.50
4	B	8025	DMS	O-S	4.44	1.80	1.50
4	D	8020	DMS	O-S	4.44	1.80	1.50
4	A	8010	DMS	O-S	4.44	1.80	1.50
4	D	8012	DMS	O-S	4.44	1.80	1.50
4	C	8024	DMS	O-S	4.44	1.80	1.50
4	A	8020	DMS	O-S	4.44	1.80	1.50
4	C	8023	DMS	O-S	4.43	1.80	1.50
4	C	8025	DMS	O-S	4.43	1.80	1.50
4	D	8018	DMS	O-S	4.43	1.80	1.50
4	D	8011	DMS	O-S	4.43	1.80	1.50
4	D	8017	DMS	O-S	4.43	1.80	1.50
4	A	8012	DMS	O-S	4.43	1.80	1.50
4	C	8032	DMS	O-S	4.42	1.80	1.50
4	A	8018	DMS	O-S	4.42	1.80	1.50
4	A	8011	DMS	O-S	4.42	1.80	1.50
4	B	8024	DMS	O-S	4.42	1.80	1.50
4	C	8009	DMS	O-S	4.41	1.80	1.50
4	B	8026	DMS	O-S	4.41	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8011	DMS	O-S	4.41	1.80	1.50
4	B	8012	DMS	O-S	4.41	1.80	1.50
4	C	8003	DMS	O-S	4.41	1.80	1.50
4	D	8009	DMS	O-S	4.41	1.80	1.50
4	C	8016	DMS	O-S	4.40	1.79	1.50
4	B	8023	DMS	O-S	4.39	1.79	1.50
4	D	8003	DMS	O-S	4.39	1.79	1.50
4	B	8014	DMS	O-S	4.38	1.79	1.50
4	C	8008	DMS	O-S	4.38	1.79	1.50
4	C	8005	DMS	O-S	4.37	1.79	1.50
4	A	8002	DMS	O-S	4.37	1.79	1.50
4	B	8005	DMS	O-S	4.37	1.79	1.50
4	C	8031	DMS	O-S	4.35	1.79	1.50
4	D	8001	DMS	O-S	4.34	1.79	1.50
4	A	8003	DMS	O-S	4.34	1.79	1.50
4	D	8002	DMS	O-S	4.34	1.79	1.50
4	A	8005	DMS	O-S	4.34	1.79	1.50
4	A	8001	DMS	O-S	4.33	1.79	1.50
4	D	8005	DMS	O-S	4.33	1.79	1.50
4	C	8002	DMS	O-S	4.32	1.79	1.50
4	C	8001	DMS	O-S	4.30	1.79	1.50
4	B	8001	DMS	O-S	4.28	1.79	1.50
4	B	8002	DMS	O-S	4.25	1.79	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8011	DMS	1	0
4	A	8022	DMS	1	0
4	A	8003	DMS	1	0
4	D	8010	DMS	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	0.01	29 (2%)	51	54	17, 30, 53, 85	0
1	B	1015/1052 (96%)	-0.08	29 (2%)	51	54	15, 26, 50, 82	0
1	C	1015/1052 (96%)	-0.06	36 (3%)	44	47	16, 26, 51, 85	0
1	D	1015/1052 (96%)	0.04	37 (3%)	42	45	17, 30, 54, 89	0
All	All	4060/4208 (96%)	-0.02	131 (3%)	47	50	15, 28, 53, 89	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	735	HIS	7.6
1	C	1023	LYS	7.5
1	B	689	GLU	7.1
1	A	735	HIS	6.8
1	D	687	GLN	6.2
1	B	731	PRO	5.8
1	D	686	PRO	5.7
1	C	689	GLU	5.7
1	B	1023	LYS	5.6
1	A	733	ALA	5.6
1	A	689	GLU	5.4
1	C	11	LEU	5.4
1	D	730	LEU	5.2
1	C	731	PRO	4.9
1	C	1022	GLN	4.9
1	A	1023	LYS	4.8
1	A	687	GLN	4.7
1	A	685	LEU	4.5
1	A	730	LEU	4.5
1	D	1023	LYS	4.4
1	D	733	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	581	ASN	4.2
1	D	689	GLU	4.2
1	C	799	THR	4.2
1	B	12	GLN	4.1
1	A	731	PRO	4.0
1	A	686	PRO	3.9
1	D	800	ARG	3.8
1	B	682	LEU	3.8
1	A	11	LEU	3.8
1	A	582	GLY	3.7
1	C	12	GLN	3.7
1	C	580	GLU	3.7
1	B	11	LEU	3.6
1	A	117	GLU	3.6
1	A	580	GLU	3.6
1	C	687	GLN	3.5
1	D	11	LEU	3.5
1	B	686	PRO	3.5
1	D	580	GLU	3.4
1	D	80	GLU	3.4
1	D	732	ALA	3.4
1	D	582	GLY	3.4
1	A	737	ILE	3.4
1	D	737	ILE	3.4
1	C	685	LEU	3.3
1	D	685	LEU	3.3
1	B	80	GLU	3.3
1	B	770	ILE	3.3
1	B	730	LEU	3.3
1	B	732	ALA	3.3
1	A	798	ALA	3.2
1	D	772	ASP	3.2
1	B	733	ALA	3.2
1	C	684	GLU	3.2
1	D	595	THR	3.1
1	A	684	GLU	3.1
1	C	735	HIS	3.1
1	C	10	VAL	3.1
1	A	732	ALA	3.1
1	A	595	THR	3.1
1	B	71	GLU	3.0
1	C	581	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	687	GLN	3.0
1	C	9	VAL	3.0
1	B	685	LEU	2.9
1	B	10	VAL	2.9
1	D	770	ILE	2.9
1	C	683	PRO	2.9
1	A	799	THR	2.9
1	B	663	LEU	2.9
1	B	735	HIS	2.9
1	D	10	VAL	2.9
1	B	684	GLU	2.8
1	A	69	VAL	2.8
1	A	79	PRO	2.8
1	D	75	GLU	2.8
1	B	9	VAL	2.7
1	C	681	GLU	2.7
1	A	800	ARG	2.7
1	B	800	ARG	2.7
1	C	730	LEU	2.7
1	C	753	ASN	2.6
1	C	686	PRO	2.6
1	D	592	PHE	2.6
1	B	683	PRO	2.6
1	C	370	GLN	2.6
1	D	684	GLU	2.5
1	C	732	ALA	2.5
1	D	578	TYR	2.5
1	D	741	THR	2.5
1	C	770	ILE	2.5
1	D	131	GLU	2.5
1	B	799	THR	2.5
1	C	667	GLU	2.4
1	D	799	THR	2.4
1	A	690	SER	2.4
1	C	669	PRO	2.4
1	B	690	SER	2.4
1	C	800	ARG	2.3
1	C	663	LEU	2.3
1	A	771	GLY	2.3
1	B	753	ASN	2.3
1	D	890	GLN	2.2
1	C	801	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	594	ASP	2.2
1	C	651	LEU	2.2
1	D	583	ASN	2.2
1	A	237	ARG	2.2
1	D	832	ASP	2.2
1	C	750	GLU	2.2
1	D	1022	GLN	2.2
1	B	681	GLU	2.2
1	A	801	ILE	2.1
1	B	737	ILE	2.1
1	A	64	PRO	2.1
1	D	891	VAL	2.1
1	D	736	ALA	2.1
1	C	595	THR	2.1
1	C	71	GLU	2.1
1	D	893	GLU	2.1
1	C	682	LEU	2.1
1	C	671	ASP	2.1
1	C	977	HIS	2.1
1	B	76	CYS	2.1
1	C	772	ASP	2.0
1	A	734	SER	2.0
1	D	12	GLN	2.0
1	D	579	ASP	2.0
1	B	653	HIS	2.0
1	A	832	ASP	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
3	NA	A	3104	1/1	0.65	0.16	50,50,50,50	0
4	DMS	B	8021	4/4	0.73	0.37	84,86,86,88	0
4	DMS	D	8021	4/4	0.73	0.38	92,93,93,94	0
4	DMS	C	8032	4/4	0.77	0.25	72,72,72,75	0
4	DMS	D	8008	4/4	0.77	0.28	87,87,87,88	0
4	DMS	C	8027	4/4	0.77	0.22	70,70,72,75	0
4	DMS	A	8007	4/4	0.78	0.35	92,92,92,93	0
4	DMS	B	8032	4/4	0.78	0.27	67,68,69,72	0
4	DMS	B	8013	4/4	0.79	0.45	95,96,96,97	0
4	DMS	A	8022	4/4	0.80	0.26	67,68,68,73	0
4	DMS	C	8004	4/4	0.80	0.27	63,64,67,70	0
4	DMS	A	8023	4/4	0.80	0.23	76,77,79,80	0
4	DMS	C	8006	4/4	0.81	0.21	56,59,60,65	0
4	DMS	C	8026	4/4	0.81	0.21	79,79,80,83	0
4	DMS	C	8025	4/4	0.82	0.25	59,60,61,62	0
4	DMS	A	8015	4/4	0.82	0.18	84,84,84,87	0
2	MG	C	3003	1/1	0.82	0.14	38,38,38,38	1
4	DMS	C	8013	4/4	0.83	0.37	88,90,90,91	0
4	DMS	B	8020	4/4	0.83	0.25	86,87,88,88	0
4	DMS	C	8030	4/4	0.83	0.22	70,73,73,74	0
4	DMS	D	8019	4/4	0.84	0.19	77,77,78,81	0
4	DMS	A	8004	4/4	0.85	0.20	57,58,62,63	0
4	DMS	B	8017	4/4	0.85	0.30	65,65,68,72	0
4	DMS	B	8014	4/4	0.87	0.23	57,60,62,63	0
4	DMS	A	8021	4/4	0.87	0.17	80,80,80,81	0
4	DMS	A	8020	4/4	0.87	0.23	58,60,62,64	0
4	DMS	C	8031	4/4	0.87	0.23	58,60,60,61	0
4	DMS	C	8029	4/4	0.88	0.17	56,57,58,65	0
3	NA	C	3104	1/1	0.88	0.23	46,46,46,46	0
4	DMS	C	8011	4/4	0.88	0.21	65,67,69,71	0
4	DMS	B	8024	4/4	0.88	0.19	66,68,69,69	0
4	DMS	B	8030	4/4	0.88	0.19	78,78,80,80	0
4	DMS	A	8009	4/4	0.88	0.30	70,72,73,73	0
4	DMS	A	8014	4/4	0.88	0.17	71,72,74,75	0
4	DMS	D	8022	4/4	0.88	0.32	74,76,77,78	0
3	NA	D	3104	1/1	0.89	0.14	49,49,49,49	0
4	DMS	D	8004	4/4	0.89	0.17	47,52,54,55	0
3	NA	B	3104	1/1	0.89	0.21	44,44,44,44	0
4	DMS	D	8012	4/4	0.89	0.28	65,67,69,69	0
4	DMS	D	8015	4/4	0.89	0.24	70,71,71,74	0
4	DMS	B	8025	4/4	0.89	0.18	68,69,71,72	0
4	DMS	B	8006	4/4	0.89	0.19	69,70,70,71	0
4	DMS	B	8007	4/4	0.89	0.15	57,59,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	C	8024	4/4	0.90	0.19	69,69,70,71	0
4	DMS	D	8014	4/4	0.90	0.18	54,56,57,57	0
4	DMS	B	8004	4/4	0.90	0.19	40,43,49,53	0
4	DMS	B	8028	4/4	0.90	0.23	92,93,93,94	0
4	DMS	C	8014	4/4	0.90	0.23	76,76,76,78	0
4	DMS	C	8018	4/4	0.90	0.20	54,57,59,59	0
2	MG	A	3003	1/1	0.91	0.09	54,54,54,54	0
4	DMS	B	8010	4/4	0.91	0.28	55,57,58,59	0
4	DMS	B	8019	4/4	0.91	0.20	66,68,69,69	0
4	DMS	A	8012	4/4	0.91	0.39	63,64,65,66	0
4	DMS	A	8019	4/4	0.92	0.18	74,76,77,77	0
4	DMS	B	8016	4/4	0.92	0.36	81,81,82,82	0
4	DMS	C	8021	4/4	0.92	0.21	52,52,53,59	0
4	DMS	C	8028	4/4	0.92	0.17	66,67,68,70	0
4	DMS	D	8007	4/4	0.92	0.15	58,58,58,60	0
4	DMS	B	8008	4/4	0.92	0.18	38,39,41,45	0
3	NA	D	3105	1/1	0.93	0.16	47,47,47,47	1
4	DMS	B	8029	4/4	0.93	0.37	86,86,86,86	0
4	DMS	C	8012	4/4	0.93	0.20	75,76,76,76	0
4	DMS	D	8009	4/4	0.93	0.20	48,49,53,53	0
4	DMS	D	8010	4/4	0.93	0.17	36,47,47,47	0
4	DMS	D	8011	4/4	0.93	0.12	49,49,51,56	0
4	DMS	A	8010	4/4	0.93	0.20	50,51,51,52	0
4	DMS	B	8031	4/4	0.93	0.17	80,81,81,82	0
2	MG	B	3001	1/1	0.93	0.07	23,23,23,23	0
4	DMS	D	8018	4/4	0.93	0.25	60,64,64,64	0
2	MG	A	3002	1/1	0.93	0.12	31,31,31,31	0
4	DMS	C	8019	4/4	0.93	0.19	76,77,77,78	0
4	DMS	C	8023	4/4	0.93	0.16	66,67,68,69	0
4	DMS	C	8017	4/4	0.94	0.17	76,76,77,78	0
4	DMS	A	8008	4/4	0.94	0.14	52,54,55,55	0
4	DMS	D	8006	4/4	0.94	0.21	68,69,70,71	0
2	MG	A	3001	1/1	0.94	0.11	29,29,29,29	0
4	DMS	B	8015	4/4	0.94	0.14	45,48,49,53	0
4	DMS	C	8022	4/4	0.94	0.23	65,66,66,67	0
4	DMS	A	8006	4/4	0.94	0.13	63,66,66,67	0
4	DMS	C	8008	4/4	0.94	0.17	45,46,47,53	0
4	DMS	C	8010	4/4	0.94	0.15	59,60,62,64	0
4	DMS	B	8027	4/4	0.94	0.12	65,66,67,67	0
4	DMS	B	8009	4/4	0.94	0.12	41,42,45,45	0
4	DMS	B	8018	4/4	0.94	0.17	73,74,74,74	0
2	MG	B	3002	1/1	0.94	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	D	8020	4/4	0.94	0.13	67,67,68,71	0
4	DMS	C	8015	4/4	0.94	0.11	74,74,75,76	0
4	DMS	C	8016	4/4	0.94	0.35	55,59,60,60	0
3	NA	D	3103	1/1	0.95	0.10	45,45,45,45	0
4	DMS	A	8017	4/4	0.95	0.12	57,59,60,61	0
4	DMS	B	8022	4/4	0.95	0.15	67,67,68,68	0
4	DMS	B	8023	4/4	0.95	0.15	54,54,55,58	0
4	DMS	B	8026	4/4	0.95	0.18	50,51,53,55	0
4	DMS	C	8007	4/4	0.95	0.13	47,48,49,49	0
4	DMS	D	8016	4/4	0.95	0.18	69,69,70,71	0
4	DMS	A	8018	4/4	0.95	0.16	67,69,69,70	0
3	NA	A	3102	1/1	0.95	0.10	22,22,22,22	0
2	MG	D	3002	1/1	0.95	0.10	33,33,33,33	0
4	DMS	A	8013	4/4	0.95	0.15	65,66,67,68	0
4	DMS	A	8003	4/4	0.95	0.18	48,48,50,55	0
4	DMS	D	8023	4/4	0.95	0.14	57,57,57,59	0
4	DMS	A	8011	4/4	0.96	0.18	48,51,52,54	0
4	DMS	D	8013	4/4	0.96	0.15	67,69,69,70	0
4	DMS	D	8002	4/4	0.96	0.12	32,36,36,38	0
4	DMS	D	8003	4/4	0.96	0.17	49,51,52,52	0
3	NA	C	3103	1/1	0.96	0.14	37,37,37,37	0
4	DMS	D	8017	4/4	0.96	0.12	68,68,69,69	0
2	MG	D	3003	1/1	0.96	0.07	52,52,52,52	0
4	DMS	C	8003	4/4	0.96	0.09	41,42,45,46	0
3	NA	B	3103	1/1	0.96	0.10	41,41,41,41	0
4	DMS	C	8020	4/4	0.96	0.19	70,70,71,71	0
3	NA	A	3103	1/1	0.96	0.11	39,39,39,39	0
4	DMS	A	8016	4/4	0.96	0.16	63,64,65,67	0
3	NA	C	3102	1/1	0.97	0.07	22,22,22,22	0
4	DMS	C	8005	4/4	0.97	0.20	41,41,43,44	0
3	NA	D	3102	1/1	0.97	0.07	24,24,24,24	0
4	DMS	A	8002	4/4	0.97	0.13	33,33,34,37	0
4	DMS	D	8001	4/4	0.97	0.09	28,31,35,37	0
4	DMS	B	8001	4/4	0.97	0.07	20,27,29,33	0
4	DMS	B	8002	4/4	0.97	0.11	27,30,30,33	0
4	DMS	B	8011	4/4	0.97	0.20	47,50,51,52	0
4	DMS	B	8003	4/4	0.97	0.11	41,43,45,45	0
2	MG	C	3002	1/1	0.97	0.10	21,21,21,21	0
4	DMS	C	8001	4/4	0.97	0.09	23,25,27,35	0
4	DMS	C	8002	4/4	0.97	0.10	26,29,32,33	0
4	DMS	B	8005	4/4	0.97	0.22	40,42,44,45	0
4	DMS	C	8009	4/4	0.98	0.12	41,43,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	D	8005	4/4	0.98	0.12	38,41,43,44	0
2	MG	C	3001	1/1	0.98	0.07	23,23,23,23	0
4	DMS	A	8005	4/4	0.98	0.14	43,44,45,46	0
3	NA	B	3102	1/1	0.98	0.10	22,22,22,22	0
4	DMS	B	8012	4/4	0.98	0.12	45,47,47,48	0
2	MG	D	3001	1/1	0.98	0.05	27,27,27,27	0
4	DMS	A	8001	4/4	0.98	0.10	25,31,33,34	0
3	NA	D	3101	1/1	0.98	0.11	35,35,35,35	0
2	MG	B	3003	1/1	0.98	0.10	50,50,50,50	0
3	NA	B	3105	1/1	0.99	0.11	12,12,12,12	1
3	NA	C	3101	1/1	0.99	0.06	26,26,26,26	0
3	NA	A	3101	1/1	0.99	0.13	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.