



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 3T0D / pdb_00003t0d
Title : E.coli (lacZ) beta-galactosidase (S796T) in complex with galactonolactone
Authors : Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.
Deposited on : 2011-07-20
Resolution : 1.93 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

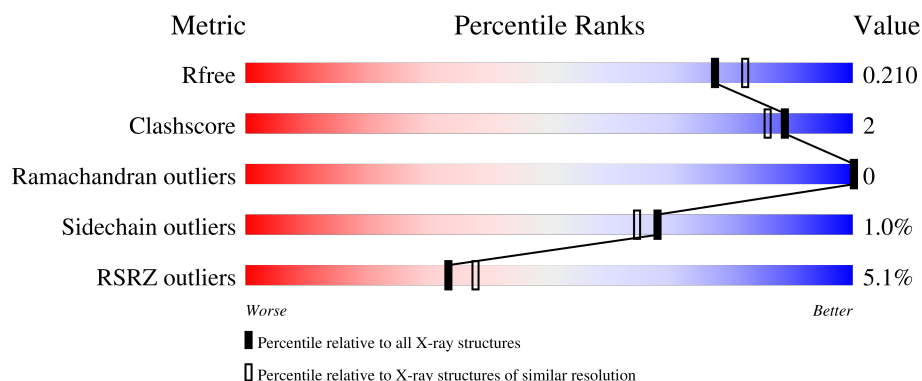
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1052	8% 90% 6%
1	B	1052	4% 91% 5%
1	C	1052	3% 91% 5%
1	D	1052	5% 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
5	DMS	B	8022	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37140 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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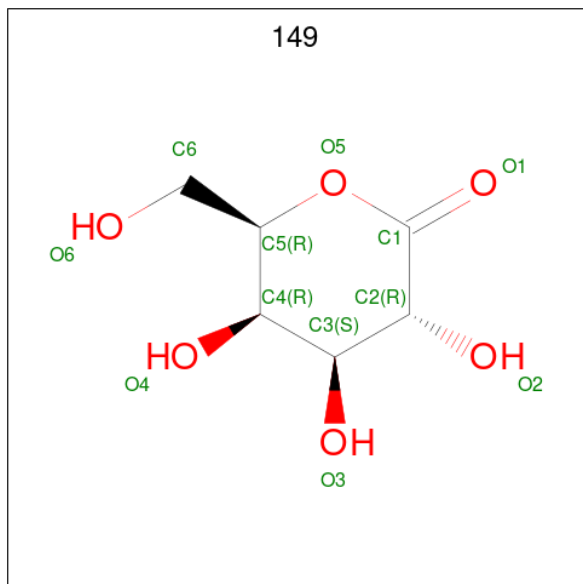
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	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 D-galactonolactone (CCD ID: 149) (formula: C₆H₁₀O₆).



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 (CCD ID: MG) (formula: Mg).

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

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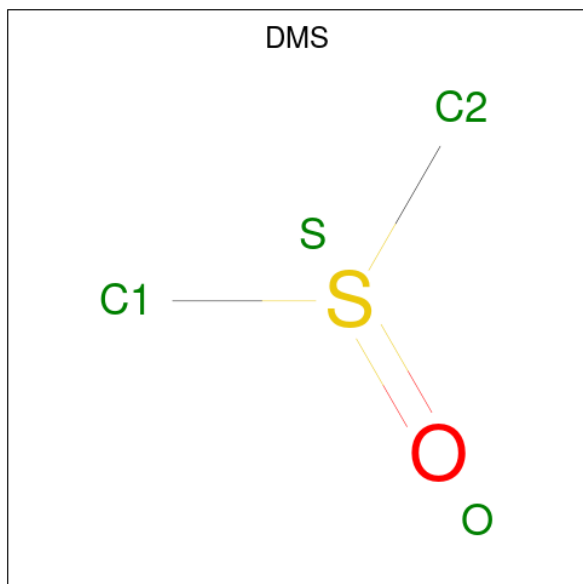
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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		

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

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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	925	Total 925	O 925	0	0
6	B	1115	Total 1115	O 1115	0	0

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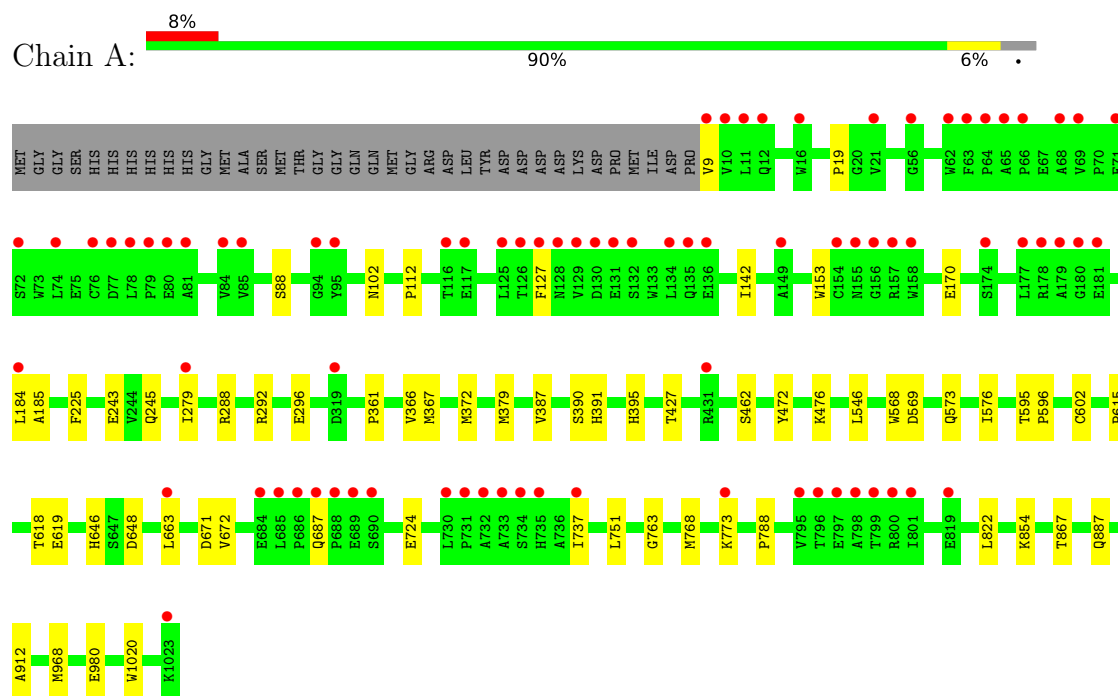
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1095	Total 1095	O 1095	0	0
6	D	884	Total 884	O 884	0	0

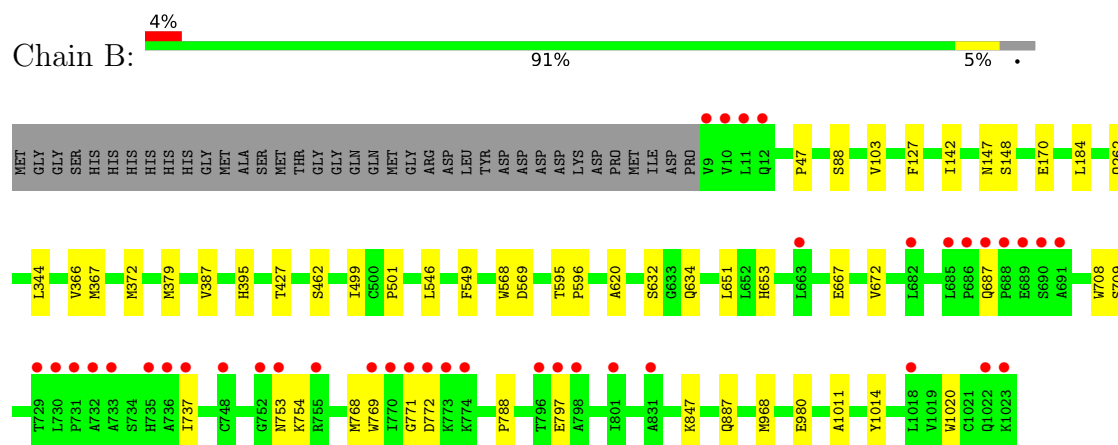
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

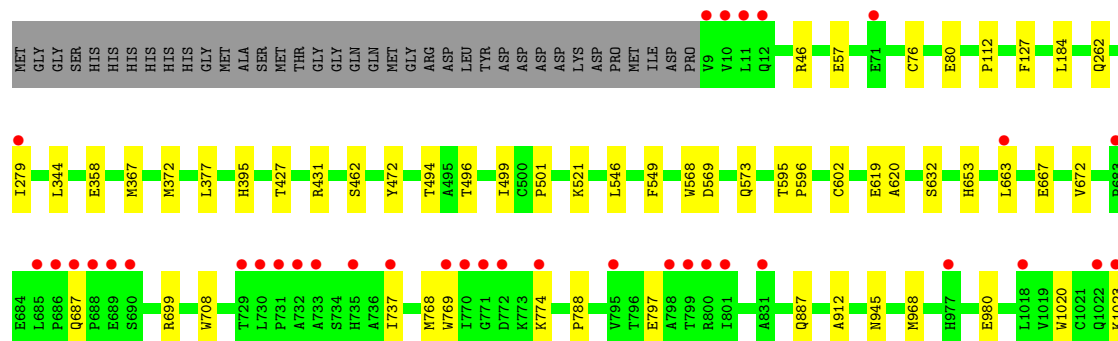
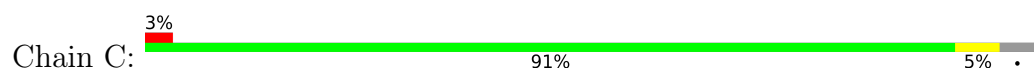
• Molecule 1: Beta-galactosidase



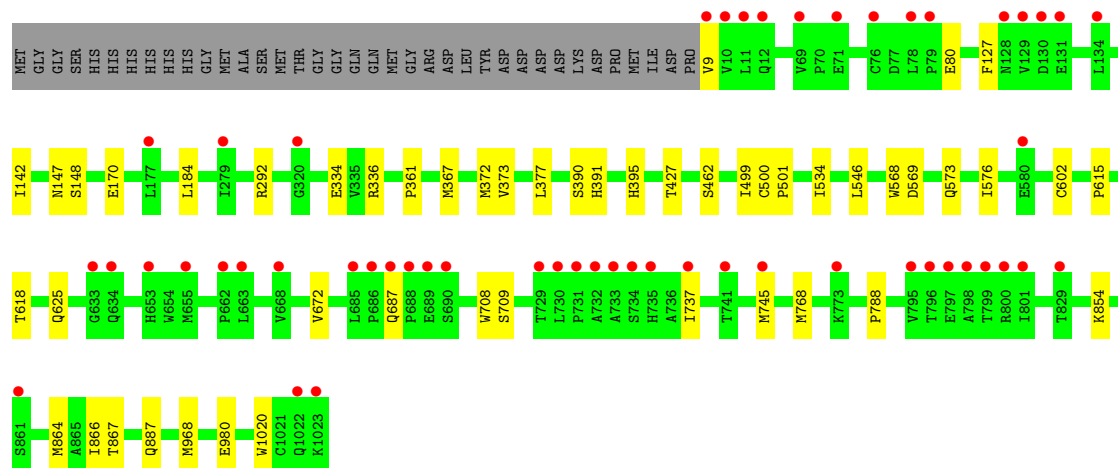
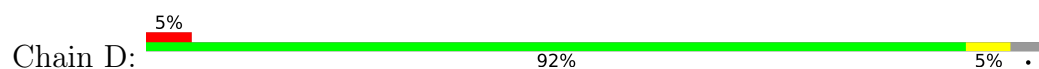
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.93Å 162.71Å 203.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.56 – 1.93 75.56 – 1.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.56-1.93) 96.4 (75.56-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.72 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.173 , 0.209 0.176 , 0.210	Depositor DCC
R_{free} test set	5190 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37140	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 40.92 % 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 2.5474e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/8400	0.67	0/11460
1	B	0.47	0/8400	0.67	0/11460
1	C	0.47	0/8400	0.67	0/11460
1	D	0.44	0/8400	0.67	0/11460
All	All	0.45	0/33600	0.67	0/45840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8158	0	7755	35	0
1	B	8158	0	7755	30	0
1	C	8158	0	7755	28	0
1	D	8158	0	7755	26	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0
3	A	2	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	88	0	132	4	0
5	B	104	0	156	7	0
5	C	120	0	180	9	0
5	D	104	0	156	4	0
6	A	925	0	0	2	0
6	B	1115	0	0	5	0
6	C	1095	0	0	3	0
6	D	884	0	0	2	0
All	All	37140	0	31680	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:HA	5:B:8022:DMS:H12	1.68	0.75
5:C:8012:DMS:H21	5:C:8025:DMS:H11	1.74	0.69
1:A:102:ASN:HD21	5:A:8019:DMS:H22	1.58	0.68
6:B:4778:HOH:O	5:C:8015:DMS:H12	1.92	0.68
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.33	0.63
1:C:887:GLN:NE2	1:C:980:GLU:O	2.32	0.62
1:A:102:ASN:ND2	5:A:8019:DMS:H22	2.15	0.61
1:D:625:GLN:HB2	5:D:8001:DMS:H21	1.83	0.59
1:C:521:LYS:HE2	6:C:4477:HOH:O	2.02	0.58
1:A:9:VAL:HG12	1:D:9:VAL:HG12	1.85	0.57
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.86	0.57
1:A:751:LEU:HD12	5:A:8018:DMS:H23	1.87	0.57
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.87	0.57
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.88	0.55
5:C:8012:DMS:C2	5:C:8025:DMS:H11	2.35	0.55
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.89	0.55
1:B:788:PRO:HD2	1:B:968:MET:HG3	1.88	0.55
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:8022:DMS:H11	6:B:4950:HOH:O	2.08	0.54
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.89	0.53
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.89	0.53
1:B:887:GLN:NE2	1:B:980:GLU:O	2.38	0.53
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.44	0.53
1:A:768:MET:HB3	6:A:4868:HOH:O	2.07	0.53
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.91	0.53
5:D:8025:DMS:H22	6:D:4545:HOH:O	2.09	0.53
1:D:373:VAL:O	1:D:377:LEU:HG	2.09	0.52
1:C:57:GLU:O	5:C:8020:DMS:H12	2.10	0.51
1:C:494:THR:O	5:C:8029:DMS:H11	2.10	0.51
1:C:653:HIS:CD2	1:C:667:GLU:HB3	2.47	0.50
1:B:427:THR:HG21	1:B:462:SER:HB3	1.93	0.50
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.46	0.50
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.47	0.49
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.47	0.49
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.95	0.49
1:D:887:GLN:NE2	1:D:980:GLU:O	2.45	0.49
1:A:773:LYS:HA	1:A:773:LYS:HD3	1.70	0.48
5:C:8008:DMS:H12	6:C:4315:HOH:O	2.13	0.48
5:D:8001:DMS:H23	6:D:4241:HOH:O	2.13	0.48
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.96	0.47
1:B:632:SER:HB2	5:B:8025:DMS:H23	1.95	0.47
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.96	0.47
1:A:615:PRO:O	1:A:618:THR:HG22	2.15	0.47
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.97	0.47
1:D:367:MET:HB3	1:D:372:MET:HE3	1.96	0.47
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.50	0.47
1:A:427:THR:HG21	1:A:462:SER:HB3	1.96	0.46
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.81	0.46
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.50	0.46
1:B:372:MET:HE2	6:B:4231:HOH:O	2.16	0.46
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.51	0.46
1:D:361:PRO:HB2	1:D:576:ILE:HG12	1.96	0.46
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.51	0.46
1:C:945:ASN:HB3	1:C:1023:LYS:HE2	1.98	0.46
1:D:427:THR:HG21	1:D:462:SER:HB3	1.97	0.46
1:A:595:THR:HA	1:A:596:PRO:C	2.41	0.45
1:A:887:GLN:NE2	1:A:980:GLU:O	2.49	0.45
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.98	0.45
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:MET:CE	1:B:395:HIS:HB3	2.46	0.45
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.98	0.45
5:B:8019:DMS:H21	6:B:4225:HOH:O	2.17	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.45
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.52	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.63	0.45
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.82	0.45
1:A:379:MET:HE1	1:A:387:VAL:HB	1.99	0.44
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.98	0.44
1:C:632:SER:HB3	5:C:8026:DMS:H12	1.99	0.44
1:C:358:GLU:HB3	1:C:367:MET:HG2	2.00	0.44
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.51	0.44
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.51	0.44
1:A:292:ARG:HH12	5:A:8010:DMS:H13	1.81	0.44
1:A:724:GLU:O	1:B:847:LYS:NZ	2.50	0.44
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.99	0.44
1:A:367:MET:HB3	1:A:372:MET:HE3	2.00	0.44
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.52	0.44
1:C:112:PRO:HG3	1:C:431:ARG:NH1	2.32	0.44
1:A:648:ASP:HB3	6:A:4883:HOH:O	2.18	0.43
1:A:390:SER:HA	1:A:391:HIS:HA	1.87	0.43
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.54	0.43
1:A:19:PRO:HD3	1:A:112:PRO:HB3	2.00	0.43
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.00	0.43
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.53	0.43
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.45	0.43
1:B:88:SER:HA	1:B:366:VAL:HG21	2.01	0.43
1:C:573:GLN:HB2	1:C:602:CYS:O	2.19	0.42
1:D:864:MET:HE3	1:D:866:ILE:HD11	2.00	0.42
1:B:47:PRO:CA	5:B:8022:DMS:H12	2.43	0.42
1:B:753:ASN:HB3	1:B:771:GLY:HA2	2.00	0.42
1:C:427:THR:HG21	1:C:462:SER:HB3	2.01	0.42
1:C:112:PRO:HG3	1:C:431:ARG:HH12	1.84	0.42
1:A:573:GLN:HB2	1:A:602:CYS:O	2.20	0.42
1:A:854:LYS:HA	1:A:867:THR:O	2.19	0.42
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.54	0.42
1:C:472:TYR:OH	5:C:8029:DMS:H12	2.20	0.42
1:A:88:SER:HA	1:A:366:VAL:HG21	2.02	0.42
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.55	0.42
1:D:292:ARG:HH12	5:D:8009:DMS:H13	1.84	0.42
1:B:595:THR:HA	1:B:596:PRO:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:854:LYS:HA	1:D:867:THR:O	2.20	0.42
1:B:754:LYS:HA	1:B:769:TRP:O	2.19	0.42
1:C:496:THR:O	5:C:8029:DMS:H13	2.19	0.42
1:B:367:MET:HB3	1:B:372:MET:HE3	2.02	0.42
1:D:573:GLN:HB2	1:D:602:CYS:O	2.20	0.42
1:B:262:GLN:HG2	6:B:5031:HOH:O	2.20	0.41
1:C:699:ARG:HD2	6:C:4995:HOH:O	2.19	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.87	0.41
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.55	0.41
1:B:379:MET:HE1	1:B:387:VAL:HB	2.03	0.41
1:C:595:THR:HA	1:C:596:PRO:C	2.45	0.41
1:A:225:PHE:HA	1:A:243:GLU:O	2.21	0.41
1:D:377:LEU:HD22	1:D:708:TRP:HA	2.03	0.41
1:D:615:PRO:O	1:D:618:THR:HG22	2.20	0.41
1:B:47:PRO:HA	5:B:8022:DMS:C1	2.45	0.41
1:A:763:GLY:HA3	1:A:822:LEU:HD13	2.02	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.41
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.56	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.21	0.40
1:B:103:VAL:CG2	5:B:8023:DMS:H13	2.50	0.40
1:B:653:HIS:CD2	1:B:667:GLU:HB3	2.56	0.40
1:A:646:HIS:NE2	1:A:671:ASP:OD1	2.53	0.40
1:C:769:TRP:NE1	1:C:774:LYS:HG2	2.36	0.40
1:D:500:CYS:HA	1:D:534:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1013/1052 (96%)	983 (97%)	30 (3%)	0	100	100
1	C	1013/1052 (96%)	986 (97%)	27 (3%)	0	100	100
1	D	1013/1052 (96%)	987 (97%)	26 (3%)	0	100	100
All	All	4052/4208 (96%)	3940 (97%)	112 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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%)	861 (99%)	7 (1%)	73	71
1	B	868/898 (97%)	860 (99%)	8 (1%)	70	67
1	C	868/898 (97%)	856 (99%)	12 (1%)	59	52
1	D	868/898 (97%)	862 (99%)	6 (1%)	76	74
All	All	3472/3592 (97%)	3439 (99%)	33 (1%)	68	64

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	ILE
1	A	296	GLU
1	A	546	LEU
1	A	663	LEU
1	A	672	VAL
1	A	687	GLN
1	A	737	ILE
1	B	344	LEU
1	B	546	LEU
1	B	634	GLN
1	B	672	VAL
1	B	687	GLN
1	B	737	ILE

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Mol	Chain	Res	Type
1	B	772	ASP
1	B	797	GLU
1	C	46	ARG
1	C	76	CYS
1	C	80	GLU
1	C	262	GLN
1	C	279	ILE
1	C	344	LEU
1	C	546	LEU
1	C	663	LEU
1	C	672	VAL
1	C	687	GLN
1	C	737	ILE
1	C	797	GLU
1	D	80	GLU
1	D	546	LEU
1	D	672	VAL
1	D	687	GLN
1	D	737	ILE
1	D	745	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	262	GLN
1	A	294	ASN
1	A	394	ASN
1	A	485	GLN
1	A	581	ASN
1	A	687	GLN
1	A	804	ASN
1	A	903	GLN
1	A	945	ASN
1	A	950	GLN
1	A	1017	GLN
1	B	49	GLN
1	B	262	GLN
1	B	266	GLN
1	B	485	GLN
1	B	624	GLN
1	B	653	HIS

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Mol	Chain	Res	Type
1	B	1017	GLN
1	C	12	GLN
1	C	49	GLN
1	C	128	ASN
1	C	365	GLN
1	C	370	GLN
1	C	394	ASN
1	C	485	GLN
1	C	624	GLN
1	C	653	HIS
1	C	844	HIS
1	D	128	ASN
1	D	266	GLN
1	D	394	ASN
1	D	485	GLN
1	D	687	GLN
1	D	903	GLN
1	D	977	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 25 are monoatomic - leaving 108 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	C	8016	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
5	DMS	A	8009	-	3,3,3	2.67	1 (33%)	3,3,3	0.45	0
5	DMS	D	8011	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	D	8014	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
5	DMS	B	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.45	0
2	149	D	2001	4	12,12,12	2.41	1 (8%)	15,17,17	0.93	1 (6%)
5	DMS	C	8012	-	3,3,3	2.66	1 (33%)	3,3,3	0.36	0
5	DMS	B	8007	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0
5	DMS	B	8010	-	3,3,3	2.68	1 (33%)	3,3,3	0.45	0
5	DMS	A	8005	-	3,3,3	2.62	1 (33%)	3,3,3	0.41	0
5	DMS	C	8009	-	3,3,3	2.62	1 (33%)	3,3,3	0.47	0
5	DMS	C	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.30	0
5	DMS	B	8012	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
5	DMS	C	8023	-	3,3,3	2.68	1 (33%)	3,3,3	0.44	0
5	DMS	C	8013	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
5	DMS	B	8018	-	3,3,3	2.72	1 (33%)	3,3,3	0.47	0
5	DMS	A	8022	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
5	DMS	D	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
5	DMS	B	8025	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
5	DMS	D	8022	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
5	DMS	A	8017	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
5	DMS	B	8016	-	3,3,3	2.72	1 (33%)	3,3,3	0.47	0
5	DMS	C	8011	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
5	DMS	A	8013	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	D	8012	-	3,3,3	2.77	1 (33%)	3,3,3	0.59	0
5	DMS	C	8028	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
5	DMS	C	8006	-	3,3,3	2.71	1 (33%)	3,3,3	0.39	0
5	DMS	D	8018	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
5	DMS	D	8020	-	3,3,3	2.70	1 (33%)	3,3,3	0.54	0
5	DMS	B	8023	-	3,3,3	2.67	1 (33%)	3,3,3	0.66	0
5	DMS	D	8021	-	3,3,3	2.71	1 (33%)	3,3,3	0.57	0
5	DMS	B	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
5	DMS	B	8013	-	3,3,3	2.77	1 (33%)	3,3,3	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8001	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
5	DMS	A	8010	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
5	DMS	B	8006	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
5	DMS	C	8025	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
5	DMS	A	8012	-	3,3,3	2.71	1 (33%)	3,3,3	0.59	0
5	DMS	D	8013	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
5	DMS	D	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
5	DMS	B	8008	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
5	DMS	A	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
5	DMS	C	8024	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	D	8026	-	3,3,3	2.70	1 (33%)	3,3,3	0.45	0
5	DMS	A	8016	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
5	DMS	A	8019	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
5	DMS	A	8021	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	C	8027	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
5	DMS	D	8009	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
5	DMS	B	8004	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
5	DMS	A	8011	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	A	8014	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	A	8015	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
5	DMS	A	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
5	DMS	A	8008	-	3,3,3	2.76	1 (33%)	3,3,3	0.53	0
5	DMS	C	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
5	DMS	C	8018	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
5	DMS	D	8023	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
5	DMS	B	8024	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
5	DMS	B	8002	-	3,3,3	2.64	1 (33%)	3,3,3	0.62	0
5	DMS	A	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
5	DMS	D	8005	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	B	8026	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
5	DMS	C	8008	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
5	DMS	A	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
5	DMS	C	8010	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
5	DMS	A	8004	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	C	8030	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8018	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
5	DMS	B	8021	-	3,3,3	2.68	1 (33%)	3,3,3	0.44	0
5	DMS	C	8029	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
5	DMS	B	8001	-	3,3,3	2.57	1 (33%)	3,3,3	0.49	0
5	DMS	C	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
5	DMS	C	8004	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
5	DMS	B	8015	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
5	DMS	A	8001	-	3,3,3	2.60	1 (33%)	3,3,3	0.56	0
5	DMS	B	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.38	0
5	DMS	C	8014	-	3,3,3	2.78	1 (33%)	3,3,3	0.66	0
2	149	C	2001	4	12,12,12	2.32	2 (16%)	15,17,17	0.97	1 (6%)
5	DMS	C	8017	-	3,3,3	2.69	1 (33%)	3,3,3	0.42	0
5	DMS	C	8022	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
5	DMS	B	8011	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
5	DMS	D	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
2	149	B	2001	4	12,12,12	2.46	2 (16%)	15,17,17	0.92	1 (6%)
5	DMS	A	8020	-	3,3,3	2.70	1 (33%)	3,3,3	0.44	0
5	DMS	C	8015	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
5	DMS	C	8002	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
5	DMS	B	8022	-	3,3,3	2.69	1 (33%)	3,3,3	0.46	0
5	DMS	C	8026	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
2	149	A	2001	4	12,12,12	2.35	2 (16%)	15,17,17	0.97	1 (6%)
5	DMS	C	8019	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
5	DMS	C	8021	-	3,3,3	2.68	1 (33%)	3,3,3	0.70	0
5	DMS	B	8009	-	3,3,3	2.63	1 (33%)	3,3,3	0.33	0
5	DMS	D	8004	-	3,3,3	2.66	1 (33%)	3,3,3	0.36	0
5	DMS	C	8020	-	3,3,3	2.68	1 (33%)	3,3,3	0.65	0
5	DMS	D	8010	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
5	DMS	B	8017	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
5	DMS	D	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.45	0
5	DMS	D	8017	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
5	DMS	B	8019	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
5	DMS	D	8015	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	D	8002	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
5	DMS	D	8024	-	3,3,3	2.74	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
5	DMS	D	8025	-	3,3,3	2.73	1 (33%)	3,3,3	0.45	0
5	DMS	D	8016	-	3,3,3	2.71	1 (33%)	3,3,3	0.49	0
5	DMS	D	8019	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
5	DMS	C	8003	-	3,3,3	2.63	1 (33%)	3,3,3	0.43	0
5	DMS	B	8014	-	3,3,3	2.67	1 (33%)	3,3,3	0.42	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	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	A	2001	4	-	1/2/22/22	0/1/1/1
2	149	D	2001	4	-	1/2/22/22	0/1/1/1

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	149	O5-C1	8.16	1.46	1.34
2	D	2001	149	O5-C1	8.05	1.46	1.34
2	A	2001	149	O5-C1	7.74	1.45	1.34
2	C	2001	149	O5-C1	7.68	1.45	1.34
5	C	8014	DMS	O-S	4.65	1.80	1.50
5	B	8024	DMS	O-S	4.65	1.80	1.50
5	B	8013	DMS	O-S	4.64	1.80	1.50
5	D	8012	DMS	O-S	4.64	1.80	1.50
5	A	8008	DMS	O-S	4.64	1.80	1.50
5	B	8007	DMS	O-S	4.64	1.80	1.50
5	D	8018	DMS	O-S	4.63	1.80	1.50
5	B	8025	DMS	O-S	4.62	1.80	1.50
5	D	8001	DMS	O-S	4.61	1.80	1.50
5	D	8023	DMS	O-S	4.60	1.80	1.50
5	D	8025	DMS	O-S	4.60	1.80	1.50
5	C	8004	DMS	O-S	4.60	1.80	1.50
5	C	8022	DMS	O-S	4.60	1.80	1.50
5	D	8024	DMS	O-S	4.60	1.80	1.50
5	B	8017	DMS	O-S	4.60	1.80	1.50
5	A	8007	DMS	O-S	4.59	1.80	1.50
5	C	8029	DMS	O-S	4.59	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8006	DMS	O-S	4.59	1.80	1.50
5	D	8019	DMS	O-S	4.59	1.80	1.50
5	A	8004	DMS	O-S	4.59	1.80	1.50
5	B	8026	DMS	O-S	4.59	1.80	1.50
5	D	8013	DMS	O-S	4.59	1.80	1.50
5	C	8013	DMS	O-S	4.58	1.80	1.50
5	B	8006	DMS	O-S	4.58	1.80	1.50
5	A	8017	DMS	O-S	4.58	1.80	1.50
5	C	8027	DMS	O-S	4.58	1.80	1.50
5	D	8015	DMS	O-S	4.58	1.80	1.50
5	C	8030	DMS	O-S	4.58	1.80	1.50
5	C	8016	DMS	O-S	4.58	1.80	1.50
5	B	8016	DMS	O-S	4.58	1.80	1.50
5	D	8005	DMS	O-S	4.58	1.80	1.50
5	A	8015	DMS	O-S	4.58	1.80	1.50
5	C	8026	DMS	O-S	4.58	1.80	1.50
5	B	8008	DMS	O-S	4.58	1.80	1.50
5	A	8006	DMS	O-S	4.58	1.80	1.50
5	A	8022	DMS	O-S	4.58	1.80	1.50
5	A	8021	DMS	O-S	4.58	1.80	1.50
5	D	8007	DMS	O-S	4.57	1.80	1.50
5	A	8013	DMS	O-S	4.57	1.80	1.50
5	C	8024	DMS	O-S	4.57	1.80	1.50
5	B	8018	DMS	O-S	4.57	1.80	1.50
5	C	8007	DMS	O-S	4.57	1.80	1.50
5	A	8018	DMS	O-S	4.57	1.80	1.50
5	D	8014	DMS	O-S	4.57	1.80	1.50
5	D	8011	DMS	O-S	4.57	1.80	1.50
5	A	8011	DMS	O-S	4.57	1.80	1.50
5	B	8012	DMS	O-S	4.56	1.80	1.50
5	D	8016	DMS	O-S	4.56	1.80	1.50
5	C	8018	DMS	O-S	4.56	1.80	1.50
5	A	8014	DMS	O-S	4.56	1.80	1.50
5	C	8019	DMS	O-S	4.56	1.80	1.50
5	C	8025	DMS	O-S	4.55	1.80	1.50
5	C	8006	DMS	O-S	4.55	1.80	1.50
5	D	8010	DMS	O-S	4.55	1.80	1.50
5	B	8019	DMS	O-S	4.55	1.80	1.50
5	D	8026	DMS	O-S	4.55	1.80	1.50
5	A	8016	DMS	O-S	4.55	1.80	1.50
5	B	8015	DMS	O-S	4.55	1.80	1.50
5	D	8017	DMS	O-S	4.55	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8010	DMS	O-S	4.54	1.80	1.50
5	A	8020	DMS	O-S	4.54	1.80	1.50
5	D	8021	DMS	O-S	4.54	1.80	1.50
5	A	8012	DMS	O-S	4.54	1.80	1.50
5	C	8008	DMS	O-S	4.54	1.80	1.50
5	D	8020	DMS	O-S	4.53	1.80	1.50
5	B	8022	DMS	O-S	4.53	1.80	1.50
5	D	8003	DMS	O-S	4.53	1.80	1.50
5	B	8004	DMS	O-S	4.52	1.80	1.50
5	C	8028	DMS	O-S	4.52	1.80	1.50
5	A	8019	DMS	O-S	4.52	1.80	1.50
5	D	8022	DMS	O-S	4.52	1.80	1.50
5	A	8003	DMS	O-S	4.51	1.80	1.50
5	C	8015	DMS	O-S	4.51	1.80	1.50
5	C	8002	DMS	O-S	4.51	1.80	1.50
5	C	8017	DMS	O-S	4.51	1.80	1.50
5	C	8023	DMS	O-S	4.50	1.79	1.50
5	C	8010	DMS	O-S	4.50	1.79	1.50
5	C	8020	DMS	O-S	4.50	1.79	1.50
5	D	8009	DMS	O-S	4.50	1.79	1.50
5	B	8021	DMS	O-S	4.50	1.79	1.50
5	B	8010	DMS	O-S	4.49	1.79	1.50
5	D	8002	DMS	O-S	4.49	1.79	1.50
5	A	8002	DMS	O-S	4.49	1.79	1.50
5	B	8014	DMS	O-S	4.49	1.79	1.50
5	B	8023	DMS	O-S	4.48	1.79	1.50
5	C	8021	DMS	O-S	4.48	1.79	1.50
5	D	8008	DMS	O-S	4.48	1.79	1.50
5	A	8009	DMS	O-S	4.48	1.79	1.50
5	C	8001	DMS	O-S	4.47	1.79	1.50
5	D	8004	DMS	O-S	4.47	1.79	1.50
5	C	8011	DMS	O-S	4.47	1.79	1.50
5	B	8003	DMS	O-S	4.46	1.79	1.50
5	C	8012	DMS	O-S	4.46	1.79	1.50
5	B	8020	DMS	O-S	4.45	1.79	1.50
5	B	8011	DMS	O-S	4.45	1.79	1.50
5	B	8002	DMS	O-S	4.44	1.79	1.50
5	C	8005	DMS	O-S	4.43	1.79	1.50
5	B	8009	DMS	O-S	4.43	1.79	1.50
5	B	8005	DMS	O-S	4.42	1.79	1.50
5	C	8003	DMS	O-S	4.42	1.79	1.50
5	A	8005	DMS	O-S	4.40	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8009	DMS	O-S	4.38	1.79	1.50
5	A	8001	DMS	O-S	4.35	1.79	1.50
5	B	8001	DMS	O-S	4.30	1.78	1.50
2	A	2001	149	O5-C5	-2.15	1.43	1.46
2	B	2001	149	O5-C5	-2.08	1.43	1.46
2	C	2001	149	O5-C5	-2.07	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	149	O5-C1-C2	3.03	123.70	119.14
2	A	2001	149	O5-C1-C2	3.01	123.67	119.14
2	C	2001	149	O5-C1-C2	2.95	123.58	119.14
2	B	2001	149	O5-C1-C2	2.87	123.45	119.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8012	DMS	2	0
5	B	8025	DMS	1	0
5	B	8023	DMS	1	0
5	D	8001	DMS	2	0
5	A	8010	DMS	1	0
5	C	8025	DMS	2	0
5	A	8019	DMS	2	0
5	D	8009	DMS	1	0
5	C	8008	DMS	1	0
5	A	8018	DMS	1	0
5	C	8029	DMS	3	0
5	C	8015	DMS	1	0
5	B	8022	DMS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8026	DMS	1	0
5	C	8020	DMS	1	0
5	B	8019	DMS	1	0
5	D	8025	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1015/1052 (96%)	0.22	81 (7%)	18	20	10, 22, 46, 79	0
1	B	1015/1052 (96%)	-0.21	39 (3%)	44	49	9, 17, 40, 77	0
1	C	1015/1052 (96%)	-0.28	36 (3%)	47	53	8, 16, 37, 79	0
1	D	1015/1052 (96%)	0.12	53 (5%)	33	37	11, 22, 43, 82	0
All	All	4060/4208 (96%)	-0.04	209 (5%)	33	38	8, 19, 42, 82	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	7.1
1	D	10	VAL	6.8
1	A	9	VAL	6.7
1	C	10	VAL	6.4
1	A	11	LEU	6.3
1	C	9	VAL	6.0
1	B	770	ILE	5.9
1	D	685	LEU	5.4
1	D	730	LEU	5.2
1	D	9	VAL	5.1
1	B	10	VAL	5.1
1	A	730	LEU	5.0
1	D	735	HIS	5.0
1	A	686	PRO	4.9
1	D	686	PRO	4.9
1	B	771	GLY	4.8
1	C	11	LEU	4.8
1	A	685	LEU	4.8
1	B	731	PRO	4.7
1	B	11	LEU	4.7
1	D	11	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	686	PRO	4.5
1	A	1023	LYS	4.4
1	C	1023	LYS	4.3
1	A	799	THR	4.3
1	B	685	LEU	4.3
1	A	798	ALA	4.3
1	C	770	ILE	4.2
1	D	799	THR	4.1
1	B	730	LEU	4.0
1	B	732	ALA	4.0
1	D	798	ALA	4.0
1	D	687	GLN	3.9
1	B	9	VAL	3.9
1	A	76	CYS	3.8
1	D	129	VAL	3.8
1	C	771	GLY	3.8
1	A	179	ALA	3.7
1	A	688	PRO	3.7
1	C	688	PRO	3.7
1	A	735	HIS	3.7
1	A	689	GLU	3.7
1	A	78	LEU	3.6
1	C	685	LEU	3.6
1	D	737	ILE	3.6
1	B	686	PRO	3.6
1	B	769	TRP	3.5
1	B	1022	GLN	3.5
1	C	730	LEU	3.5
1	B	735	HIS	3.5
1	A	130	ASP	3.5
1	B	753	ASN	3.5
1	C	733	ALA	3.5
1	A	733	ALA	3.4
1	D	732	ALA	3.4
1	C	798	ALA	3.4
1	A	687	GLN	3.4
1	D	688	PRO	3.4
1	D	731	PRO	3.4
1	A	117	GLU	3.3
1	B	1023	LYS	3.3
1	C	1022	GLN	3.3
1	C	772	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	733	ALA	3.3
1	A	177	LEU	3.3
1	B	772	ASP	3.3
1	D	800	ARG	3.3
1	A	136	GLU	3.2
1	B	737	ILE	3.2
1	B	689	GLU	3.2
1	A	84	VAL	3.2
1	C	799	THR	3.2
1	B	688	PRO	3.2
1	D	1023	LYS	3.2
1	C	690	SER	3.1
1	A	180	GLY	3.1
1	A	129	VAL	3.1
1	D	795	VAL	3.1
1	A	63	PHE	3.1
1	A	80	GLU	3.1
1	C	800	ARG	3.0
1	A	319	ASP	3.0
1	D	663	LEU	3.0
1	A	85	VAL	3.0
1	A	127	PHE	3.0
1	D	79	PRO	3.0
1	A	65	ALA	3.0
1	A	663	LEU	3.0
1	A	69	VAL	3.0
1	C	12	GLN	3.0
1	C	683	PRO	2.9
1	B	773	LYS	2.9
1	A	737	ILE	2.9
1	A	796	THR	2.9
1	A	72	SER	2.9
1	D	733	ALA	2.8
1	D	634	GLN	2.8
1	D	130	ASP	2.8
1	A	81	ALA	2.8
1	A	731	PRO	2.8
1	D	689	GLU	2.8
1	B	12	GLN	2.8
1	A	801	ILE	2.8
1	C	831	ALA	2.7
1	C	731	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	128	ASN	2.7
1	A	773	LYS	2.7
1	D	76	CYS	2.7
1	B	796	THR	2.7
1	B	690	SER	2.7
1	B	797	GLU	2.7
1	A	795	VAL	2.7
1	D	320	GLY	2.7
1	B	736	ALA	2.6
1	A	431	ARG	2.6
1	C	687	GLN	2.6
1	B	729	THR	2.6
1	C	735	HIS	2.6
1	D	745	MET	2.6
1	A	181	GLU	2.6
1	B	774	LYS	2.6
1	A	79	PRO	2.6
1	D	71	GLU	2.6
1	D	131	GLU	2.6
1	C	732	ALA	2.6
1	C	689	GLU	2.6
1	A	68	ALA	2.6
1	A	77	ASP	2.5
1	B	663	LEU	2.5
1	D	690	SER	2.5
1	D	1022	GLN	2.5
1	A	128	ASN	2.5
1	B	755	ARG	2.5
1	A	71	GLU	2.5
1	C	769	TRP	2.5
1	A	732	ALA	2.5
1	D	773	LYS	2.4
1	A	800	ARG	2.4
1	D	655	MET	2.4
1	B	801	ILE	2.4
1	A	16	TRP	2.4
1	A	62	TRP	2.4
1	D	12	GLN	2.4
1	A	94	GLY	2.4
1	A	74	LEU	2.4
1	C	1018	LEU	2.4
1	D	78	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	2.4
1	D	279	ILE	2.4
1	B	798	ALA	2.4
1	D	653	HIS	2.4
1	C	774	LYS	2.4
1	A	126	THR	2.3
1	A	149	ALA	2.3
1	B	831	ALA	2.3
1	A	56	GLY	2.3
1	B	682	LEU	2.3
1	D	829	THR	2.3
1	D	861	SER	2.3
1	A	21	VAL	2.3
1	A	131	GLU	2.3
1	A	132	SER	2.3
1	A	116	THR	2.3
1	A	134	LEU	2.3
1	A	66	PRO	2.2
1	A	819	GLU	2.2
1	A	174	SER	2.2
1	D	69	VAL	2.2
1	B	748	CYS	2.2
1	A	734	SER	2.2
1	D	734	SER	2.2
1	D	796	THR	2.2
1	A	135	GLN	2.2
1	D	177	LEU	2.2
1	B	752	GLY	2.2
1	A	157	ARG	2.2
1	C	795	VAL	2.2
1	C	663	LEU	2.2
1	D	797	GLU	2.1
1	B	687	GLN	2.1
1	A	690	SER	2.1
1	A	156	GLY	2.1
1	D	134	LEU	2.1
1	C	977	HIS	2.1
1	C	737	ILE	2.1
1	A	684	GLU	2.1
1	A	155	ASN	2.1
1	B	1018	LEU	2.1
1	D	801	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	797	GLU	2.1
1	C	71	GLU	2.1
1	C	729	THR	2.1
1	D	580	GLU	2.1
1	D	633	GLY	2.1
1	A	158	TRP	2.1
1	A	125	LEU	2.1
1	A	184	LEU	2.1
1	A	279	ILE	2.0
1	C	279	ILE	2.0
1	C	801	ILE	2.0
1	D	741	THR	2.0
1	A	64	PRO	2.0
1	D	662	PRO	2.0
1	A	154	CYS	2.0
1	B	691	ALA	2.0
1	A	12	GLN	2.0
1	D	729	THR	2.0
1	A	95	TYR	2.0
1	D	668	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8018	4/4	0.60	0.39	87,88,89,89	0
5	DMS	D	8012	4/4	0.71	0.32	73,75,75,77	0
5	DMS	D	8023	4/4	0.71	0.29	61,63,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	8007	4/4	0.72	0.32	82,82,82,83	0
5	DMS	A	8014	4/4	0.73	0.27	67,68,69,69	0
5	DMS	D	8014	4/4	0.74	0.25	68,69,69,70	0
5	DMS	D	8019	4/4	0.74	0.31	75,75,76,76	0
5	DMS	B	8008	4/4	0.74	0.30	63,63,63,64	0
5	DMS	C	8019	4/4	0.75	0.29	57,58,61,62	0
4	NA	B	3104	1/1	0.75	0.21	43,43,43,43	0
5	DMS	C	8014	4/4	0.75	0.23	49,50,52,60	0
5	DMS	C	8027	4/4	0.76	0.27	74,74,75,76	0
5	DMS	B	8017	4/4	0.77	0.26	72,74,75,76	0
4	NA	D	3104	1/1	0.77	0.20	43,43,43,43	0
5	DMS	D	8015	4/4	0.78	0.33	85,85,86,86	0
5	DMS	B	8011	4/4	0.78	0.29	57,57,58,61	0
5	DMS	B	8024	4/4	0.78	0.23	48,49,51,55	0
3	MG	B	3004	1/1	0.80	0.19	46,46,46,46	0
5	DMS	D	8017	4/4	0.81	0.25	66,69,69,69	0
5	DMS	A	8021	4/4	0.81	0.24	59,61,63,66	0
5	DMS	D	8013	4/4	0.81	0.25	63,65,66,68	0
5	DMS	A	8011	4/4	0.82	0.26	69,69,69,71	0
5	DMS	C	8022	4/4	0.82	0.22	54,56,58,61	0
5	DMS	C	8026	4/4	0.82	0.25	61,64,64,65	0
3	MG	A	3002	1/1	0.82	0.11	26,26,26,26	0
5	DMS	D	8018	4/4	0.82	0.21	50,50,50,56	0
5	DMS	A	8018	4/4	0.82	0.24	59,60,61,62	0
5	DMS	B	8016	4/4	0.82	0.32	71,71,72,73	0
5	DMS	C	8006	4/4	0.83	0.23	46,47,47,50	0
5	DMS	B	8020	4/4	0.83	0.26	52,54,54,56	0
5	DMS	B	8013	4/4	0.83	0.18	47,49,52,57	0
5	DMS	D	8024	4/4	0.83	0.24	64,64,64,66	0
5	DMS	C	8030	4/4	0.84	0.20	68,69,69,69	0
5	DMS	D	8005	4/4	0.84	0.24	62,64,66,66	0
5	DMS	B	8026	4/4	0.84	0.20	58,60,60,63	0
5	DMS	C	8018	4/4	0.84	0.20	41,45,47,52	0
5	DMS	B	8025	4/4	0.85	0.22	58,59,59,60	0
5	DMS	C	8029	4/4	0.85	0.18	47,48,48,53	0
5	DMS	D	8011	4/4	0.85	0.18	52,54,55,58	0
5	DMS	A	8015	4/4	0.85	0.21	54,57,58,59	0
5	DMS	A	8016	4/4	0.86	0.26	69,69,69,69	0
5	DMS	A	8004	4/4	0.86	0.19	39,40,44,45	0
5	DMS	A	8012	4/4	0.86	0.22	58,59,59,61	0
5	DMS	C	8025	4/4	0.86	0.19	46,48,49,52	0
5	DMS	A	8022	4/4	0.86	0.23	57,57,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8008	4/4	0.87	0.19	49,51,53,56	0
5	DMS	B	8006	4/4	0.87	0.19	37,42,44,44	0
5	DMS	C	8016	4/4	0.87	0.20	56,57,58,58	0
4	NA	A	3104	1/1	0.87	0.15	37,37,37,37	0
5	DMS	D	8020	4/4	0.87	0.21	47,48,49,53	0
5	DMS	A	8020	4/4	0.87	0.23	60,61,61,62	0
5	DMS	C	8021	4/4	0.87	0.21	45,47,47,48	0
5	DMS	D	8026	4/4	0.87	0.21	53,55,56,57	0
5	DMS	A	8013	4/4	0.88	0.20	67,68,68,69	0
5	DMS	B	8012	4/4	0.88	0.21	59,60,62,62	0
5	DMS	A	8007	4/4	0.88	0.20	57,61,62,62	0
5	DMS	B	8019	4/4	0.88	0.19	57,58,58,59	0
5	DMS	B	8015	4/4	0.88	0.20	55,56,58,59	0
5	DMS	D	8010	4/4	0.89	0.19	65,67,67,68	0
3	MG	D	3002	1/1	0.89	0.10	24,24,24,24	0
5	DMS	D	8016	4/4	0.89	0.18	48,50,51,53	0
5	DMS	C	8012	4/4	0.89	0.18	32,34,36,42	0
5	DMS	B	8021	4/4	0.89	0.20	49,51,52,52	0
5	DMS	D	8022	4/4	0.90	0.15	35,36,37,44	0
5	DMS	C	8011	4/4	0.90	0.21	44,45,46,48	0
5	DMS	C	8028	4/4	0.91	0.17	40,42,43,46	0
5	DMS	D	8021	4/4	0.91	0.16	49,49,50,51	0
4	NA	A	3103	1/1	0.91	0.09	39,39,39,39	0
3	MG	B	3001	1/1	0.91	0.05	13,13,13,13	0
5	DMS	C	8020	4/4	0.91	0.14	27,34,35,40	0
5	DMS	B	8023	4/4	0.91	0.21	45,46,47,48	0
5	DMS	B	8022	4/4	0.92	0.13	24,25,31,32	0
3	MG	A	3001	1/1	0.92	0.04	18,18,18,18	0
5	DMS	A	8017	4/4	0.92	0.15	57,58,59,59	0
5	DMS	C	8017	4/4	0.92	0.15	32,35,36,38	0
4	NA	C	3104	1/1	0.92	0.09	26,26,26,26	0
5	DMS	D	8003	4/4	0.92	0.12	27,30,35,35	0
5	DMS	A	8008	4/4	0.93	0.15	39,39,39,41	0
5	DMS	A	8019	4/4	0.93	0.14	39,40,41,44	0
5	DMS	B	8002	4/4	0.93	0.12	24,24,26,27	0
4	NA	D	3103	1/1	0.93	0.09	34,34,34,34	0
5	DMS	C	8013	4/4	0.93	0.14	55,55,56,56	0
5	DMS	C	8002	4/4	0.93	0.10	21,21,29,29	0
5	DMS	C	8024	4/4	0.93	0.16	55,56,56,56	0
5	DMS	D	8025	4/4	0.93	0.14	44,45,46,51	0
5	DMS	C	8004	4/4	0.93	0.15	33,37,39,40	0
4	NA	B	3102	1/1	0.94	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8023	4/4	0.94	0.14	45,46,46,47	0
5	DMS	A	8006	4/4	0.94	0.14	50,50,52,52	0
5	DMS	B	8014	4/4	0.94	0.12	35,38,39,41	0
4	NA	B	3103	1/1	0.94	0.09	30,30,30,30	0
5	DMS	C	8007	4/4	0.94	0.12	39,39,40,41	0
5	DMS	B	8007	4/4	0.94	0.12	32,32,35,36	0
3	MG	D	3001	1/1	0.94	0.04	18,18,18,18	0
5	DMS	A	8002	4/4	0.94	0.16	28,29,30,33	0
5	DMS	D	8001	4/4	0.94	0.16	30,32,32,36	0
4	NA	C	3102	1/1	0.95	0.06	16,16,16,16	0
3	MG	B	3002	1/1	0.95	0.09	14,14,14,14	0
5	DMS	D	8002	4/4	0.95	0.13	32,33,34,35	0
3	MG	C	3001	1/1	0.95	0.06	11,11,11,11	0
4	NA	A	3101	1/1	0.95	0.05	18,18,18,18	0
5	DMS	A	8010	4/4	0.95	0.13	42,43,44,45	0
5	DMS	D	8009	4/4	0.95	0.11	36,39,40,40	0
3	MG	C	3002	1/1	0.95	0.06	16,16,16,16	0
5	DMS	A	8005	4/4	0.96	0.10	30,31,32,34	0
5	DMS	D	8006	4/4	0.96	0.11	40,42,42,44	0
4	NA	C	3103	1/1	0.96	0.06	26,26,26,26	0
5	DMS	D	8008	4/4	0.96	0.10	34,35,35,37	0
5	DMS	B	8010	4/4	0.96	0.10	35,36,37,39	0
5	DMS	C	8010	4/4	0.96	0.11	33,35,36,37	0
5	DMS	A	8003	4/4	0.96	0.10	23,29,29,30	0
2	149	D	2001	12/12	0.96	0.06	15,18,20,22	0
5	DMS	B	8004	4/4	0.96	0.09	18,22,24,29	0
5	DMS	A	8009	4/4	0.96	0.10	36,36,37,38	0
5	DMS	C	8015	4/4	0.96	0.13	40,42,42,44	0
5	DMS	B	8001	4/4	0.97	0.07	16,20,22,24	0
5	DMS	C	8009	4/4	0.97	0.07	20,21,22,22	0
2	149	A	2001	12/12	0.97	0.05	14,18,22,25	0
5	DMS	C	8005	4/4	0.97	0.10	29,30,30,33	0
2	149	B	2001	12/12	0.97	0.05	8,11,16,16	0
5	DMS	B	8005	4/4	0.97	0.09	31,31,31,31	0
4	NA	C	3101	1/1	0.98	0.03	10,10,10,10	0
2	149	C	2001	12/12	0.98	0.05	10,12,15,16	0
5	DMS	B	8003	4/4	0.98	0.08	26,26,27,29	0
5	DMS	C	8001	4/4	0.98	0.06	14,15,18,21	0
5	DMS	D	8004	4/4	0.98	0.08	31,31,33,34	0
5	DMS	B	8009	4/4	0.98	0.08	25,28,32,34	0
5	DMS	C	8003	4/4	0.98	0.07	22,25,27,28	0
5	DMS	A	8001	4/4	0.98	0.07	16,22,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	3101	1/1	0.98	0.05	18,18,18,18	0
4	NA	B	3101	1/1	0.99	0.06	13,13,13,13	0
4	NA	D	3102	1/1	0.99	0.03	16,16,16,16	0
4	NA	A	3102	1/1	0.99	0.02	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.