



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:56 PM GMT

PDB ID : 4DUW
Title : E. coli (lacZ) beta-galactosidase (G974A) in complex with allolactose
Authors : Wheatley, R.W.; Lo, S.; Janzcewicz, L.J.; Dugdale, M.L.; Huber, R.E.
Deposited on : 2012-02-22
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

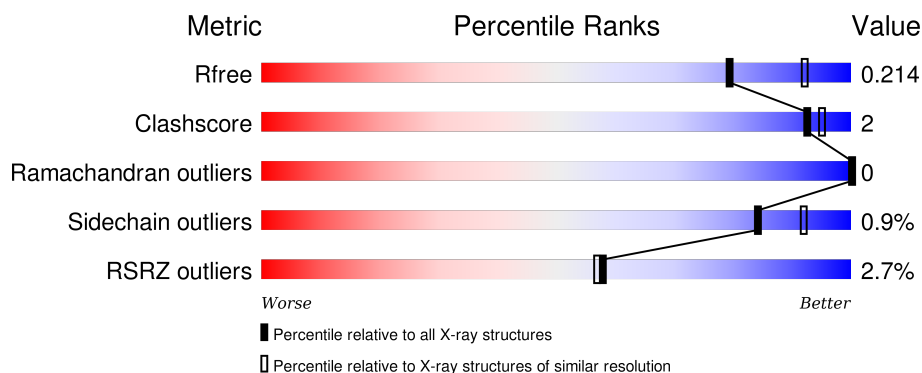
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	B	1052	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	C	1052	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	1052	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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
2	LAK	A	2001	-	-	-	X
2	LAK	C	2001	-	-	-	X
2	LAK	D	2001	-	-	-	X
3	MG	D	3002	-	-	-	X
4	NA	B	3103	-	-	-	X
4	NA	C	3101	-	-	-	X
5	DMS	A	8003	-	-	-	X
5	DMS	A	8004	-	-	-	X
5	DMS	A	8006	-	-	-	X
5	DMS	A	8014	-	-	-	X
5	DMS	A	8015	-	-	-	X
5	DMS	A	8017	-	-	-	X
5	DMS	A	8018	-	-	-	X
5	DMS	B	8004	-	-	-	X
5	DMS	B	8005	-	-	-	X
5	DMS	B	8006	-	-	-	X
5	DMS	B	8013	-	-	-	X
5	DMS	B	8016	-	-	-	X
5	DMS	B	8019	-	-	-	X
5	DMS	B	8021	-	-	-	X
5	DMS	B	8023	-	-	-	X
5	DMS	C	8003	-	-	-	X
5	DMS	C	8004	-	-	-	X
5	DMS	C	8013	-	-	-	X
5	DMS	C	8015	-	-	-	X
5	DMS	C	8016	-	-	-	X
5	DMS	C	8020	-	-	-	X
5	DMS	D	8002	-	-	X	X
5	DMS	D	8004	-	-	-	X
5	DMS	D	8012	-	-	-	X
5	DMS	D	8015	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36668 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	-	INITIATING METHIONINE	UNP P00722
A	-27	GLY	-	EXPRESSION TAG	UNP P00722
A	-26	GLY	-	EXPRESSION TAG	UNP P00722
A	-25	SER	-	EXPRESSION TAG	UNP P00722
A	-24	HIS	-	EXPRESSION TAG	UNP P00722
A	-23	HIS	-	EXPRESSION TAG	UNP P00722
A	-22	HIS	-	EXPRESSION TAG	UNP P00722
A	-21	HIS	-	EXPRESSION TAG	UNP P00722
A	-20	HIS	-	EXPRESSION TAG	UNP P00722
A	-19	HIS	-	EXPRESSION TAG	UNP P00722
A	-18	GLY	-	EXPRESSION TAG	UNP P00722
A	-17	MET	-	EXPRESSION TAG	UNP P00722
A	-16	ALA	-	EXPRESSION TAG	UNP P00722
A	-15	SER	-	EXPRESSION TAG	UNP P00722
A	-14	MET	-	EXPRESSION TAG	UNP P00722
A	-13	THR	-	EXPRESSION TAG	UNP P00722
A	-12	GLY	-	EXPRESSION TAG	UNP P00722
A	-11	GLY	-	EXPRESSION TAG	UNP P00722
A	-10	GLN	-	EXPRESSION TAG	UNP P00722
A	-9	GLN	-	EXPRESSION TAG	UNP P00722
A	-8	MET	-	EXPRESSION TAG	UNP P00722

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

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

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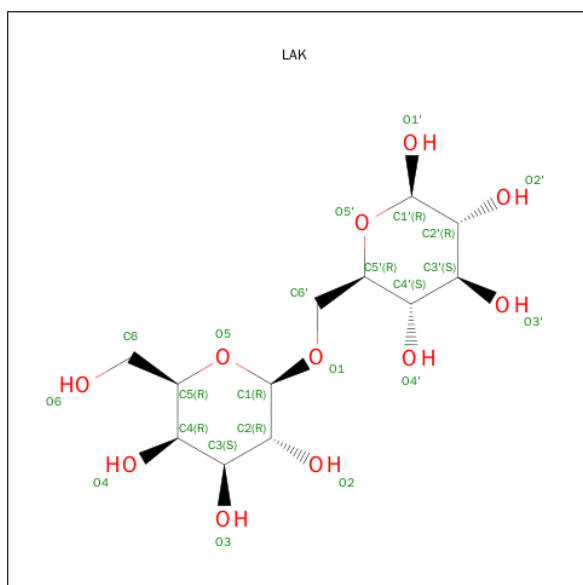
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	EXPRESSION TAG	UNP P00722
C	2	LYS	-	EXPRESSION TAG	UNP P00722
C	3	ASP	-	EXPRESSION TAG	UNP P00722
C	4	PRO	-	EXPRESSION TAG	UNP P00722
C	5	MET	-	EXPRESSION TAG	UNP P00722
C	6	ILE	-	EXPRESSION TAG	UNP P00722
C	7	ASP	-	EXPRESSION TAG	UNP P00722
C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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	EXPRESSION TAG	UNP P00722
D	6	ILE	-	EXPRESSION TAG	UNP P00722
D	7	ASP	-	EXPRESSION TAG	UNP P00722
D	8	PRO	-	EXPRESSION TAG	UNP P00722
D	794	ALA	GLY	ENGINEERED MUTATION	UNP P00722

- Molecule 2 is SUGAR (BETA-D-GALACTOPYRANOSYL-1-6-BETA-D-GLUCOPYRANOSE) (three-letter code: LAK) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

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

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

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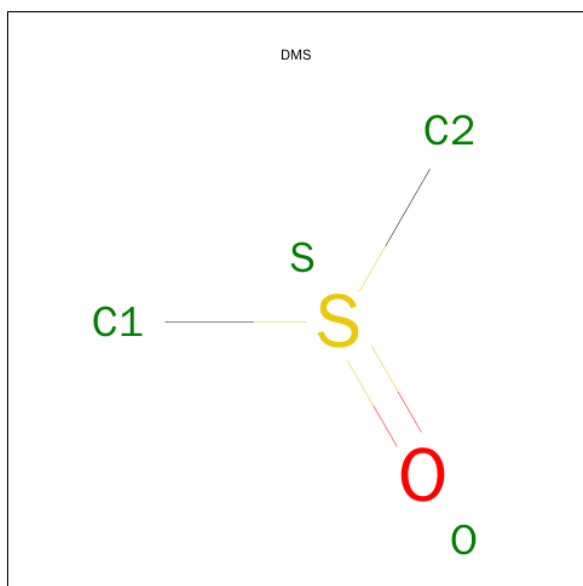
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: 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	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	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	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	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

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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

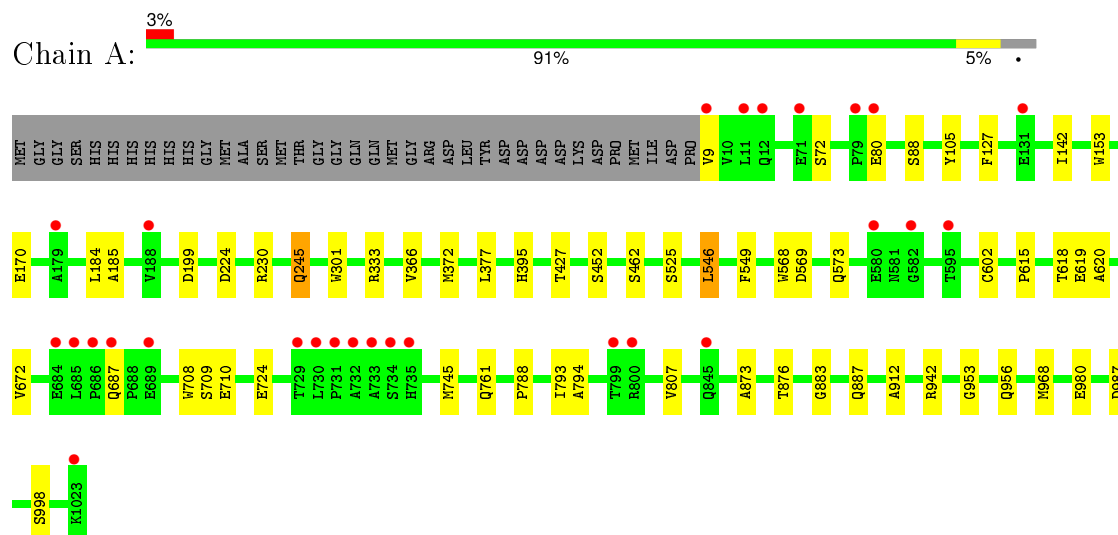
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	824	Total 824	O 824	0	0
6	B	997	Total 997	O 997	0	0
6	C	976	Total 976	O 976	0	0
6	D	813	Total 813	O 813	0	0

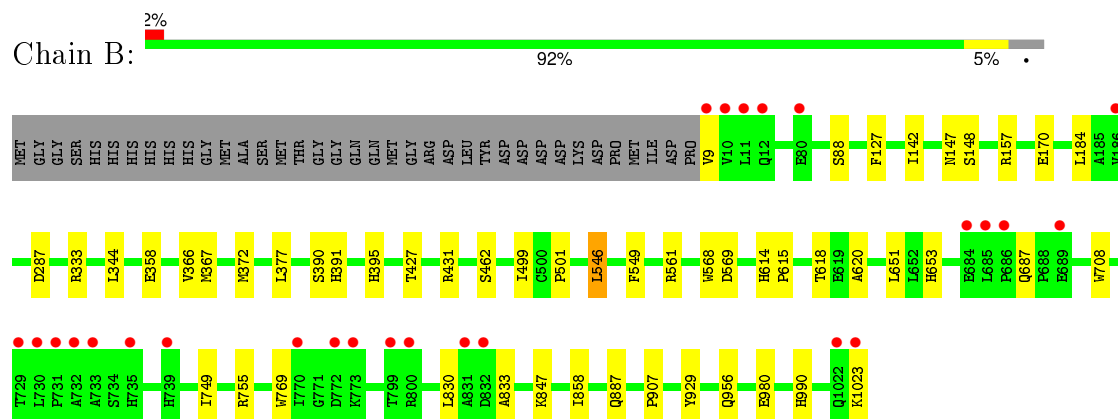
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

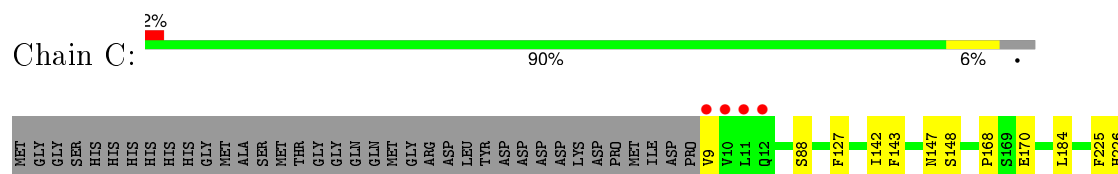
• Molecule 1: Beta-galactosidase

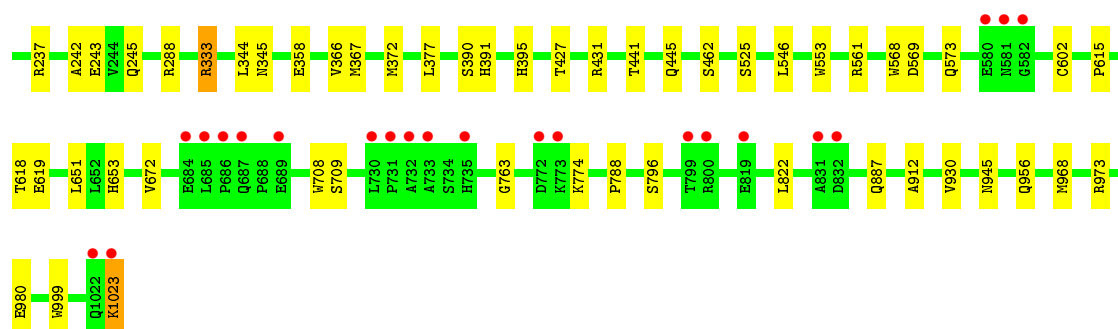


• Molecule 1: Beta-galactosidase

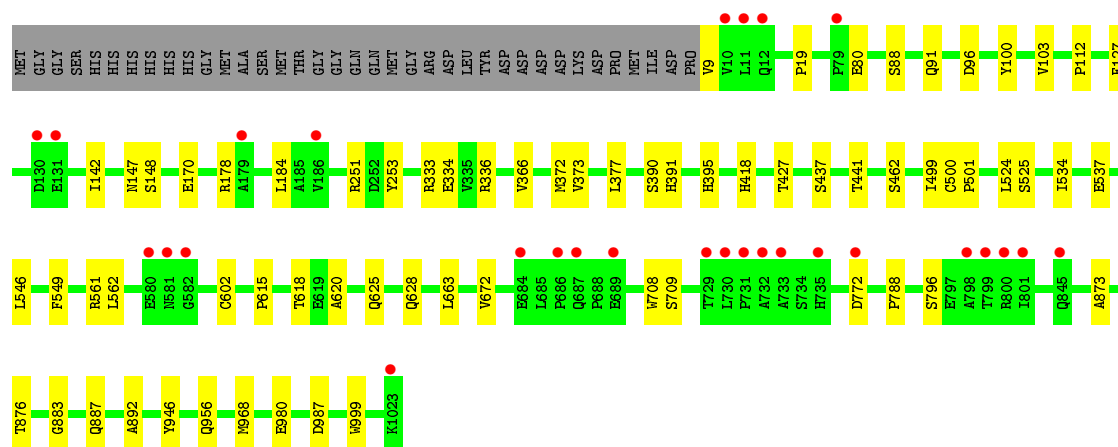
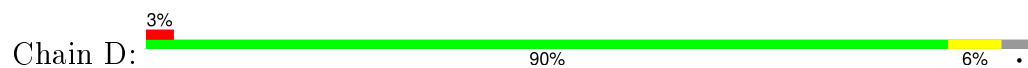


• Molecule 1: Beta-galactosidase





• 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	151.83Å 162.63Å 203.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.81 – 2.20 24.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.81-2.20) 92.6 (24.82-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.213 0.163 , 0.214	Depositor DCC
R_{free} test set	3378 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 235390 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36668	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 40.88 % 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 2.5641e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, DMS, LAK

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/8400	0.54	0/11460
1	B	0.40	0/8400	0.54	0/11460
1	C	0.40	0/8400	0.54	1/11460 (0.0%)
1	D	0.38	0/8400	0.53	0/11460
All	All	0.39	0/33600	0.54	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(°)	Ideal(°)
1	C	553	TRP	CA-CB-CG	-5.09	104.03	113.70

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	32	0
1	B	8158	0	7755	31	0
1	C	8158	0	7755	33	0
1	D	8158	0	7755	36	0
2	A	23	0	21	0	0
2	B	23	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	23	0	21	0	0
2	D	23	0	21	1	0
3	A	3	0	0	0	0
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	72	0	108	1	0
5	B	96	0	144	0	0
5	C	80	0	120	1	0
5	D	60	0	90	4	0
6	A	824	0	0	1	0
6	B	997	0	0	6	0
6	C	976	0	0	1	0
6	D	813	0	0	1	0
All	All	36668	0	31566	130	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 (130) 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:142:ILE:HG12	1:B:170:GLU:HG2	1.69	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.72	0.72
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.73	0.71
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.73	0.69
5:D:8002:DMS:H22	6:D:4227:HOH:O	1.94	0.66
1:B:887:GLN:NE2	1:B:980:GLU:O	2.30	0.65
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.80	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.30	0.64
1:C:887:GLN:NE2	1:C:980:GLU:O	2.32	0.63
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.36	0.61
1:A:887:GLN:NE2	1:A:980:GLU:O	2.33	0.60
1:D:628:GLN:OE1	5:D:8002:DMS:H21	2.04	0.57
1:B:749:ILE:HD13	1:B:858:ILE:HD12	1.86	0.56
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.41	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HG21	1:A:462:SER:HB3	1.90	0.54
1:D:19:PRO:HD3	1:D:112:PRO:HB3	1.90	0.54
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.73	0.54
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.44	0.53
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.91	0.53
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.90	0.53
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.91	0.53
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.91	0.53
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.44	0.52
1:B:755:ARG:HB2	1:B:769:TRP:HB2	1.91	0.52
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.45	0.52
1:C:945:ASN:HB3	1:C:1023:LYS:HE2	1.91	0.52
1:A:724:GLU:O	1:B:847:LYS:NZ	2.42	0.52
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.45	0.52
1:B:615:PRO:O	1:B:618:THR:HG22	2.10	0.52
1:D:427:THR:HG21	1:D:462:SER:HB3	1.91	0.51
1:D:500:CYS:HA	1:D:534:ILE:O	2.11	0.51
1:D:373:VAL:O	1:D:377:LEU:HG	2.10	0.51
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.50
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.94	0.50
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.94	0.50
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.47	0.49
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.94	0.49
1:C:88:SER:HA	1:C:366:VAL:HG21	1.94	0.48
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.95	0.48
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.42	0.48
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.42	0.48
1:B:9:VAL:HG22	1:C:9:VAL:HG22	1.95	0.48
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.95	0.48
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.49	0.48
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.77	0.48
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.49	0.48
1:C:573:GLN:HB2	1:C:602:CYS:O	2.13	0.47
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.96	0.47
1:C:441:THR:O	1:C:445:GLN:HG3	2.15	0.47
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.96	0.47
1:A:873:ALA:O	1:A:876:THR:HG22	2.15	0.47
1:B:367:MET:HE2	1:B:372:MET:HG3	1.96	0.47
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.95	0.47
1:C:615:PRO:O	1:C:618:THR:HG22	2.15	0.47
1:A:794:ALA:HA	1:A:998:SER:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HD3	6:B:4651:HOH:O	2.15	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:D:390:SER:HA	1:D:391:HIS:HA	1.77	0.46
1:C:561:ARG:HD3	1:D:525:SER:O	2.15	0.46
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.50	0.46
1:A:573:GLN:HB2	1:A:602:CYS:O	2.16	0.46
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.98	0.46
1:A:88:SER:HA	1:A:366:VAL:HG21	1.98	0.46
1:C:796:SER:HB3	1:C:999:TRP:HB3	1.98	0.46
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.45
6:B:4674:HOH:O	5:C:8013:DMS:H11	2.15	0.45
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.69	0.45
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.46	0.45
1:A:546:LEU:HA	6:A:4125:HOH:O	2.17	0.45
1:A:745:MET:HA	1:A:761:GLN:HE21	1.82	0.45
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.81	0.45
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.98	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.66	0.44
1:C:427:THR:HG21	1:C:462:SER:HB3	2.00	0.44
1:D:625:GLN:HB2	5:D:8002:DMS:H23	1.98	0.44
1:D:88:SER:HA	1:D:366:VAL:HG21	1.99	0.44
1:D:537:GLU:OE2	2:D:2001:LAK:H1	2.17	0.44
1:D:615:PRO:O	1:D:618:THR:HG22	2.17	0.44
1:A:9:VAL:HG12	1:D:9:VAL:HG12	2.00	0.44
1:C:525:SER:O	1:D:561:ARG:HD3	2.18	0.44
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.44
1:B:431:ARG:HB2	6:B:4879:HOH:O	2.17	0.44
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.01	0.43
1:B:427:THR:HG21	1:B:462:SER:HB3	2.00	0.43
1:D:437:SER:O	1:D:441:THR:HG23	2.18	0.43
1:D:796:SER:HB3	1:D:999:TRP:HB3	2.01	0.43
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.99	0.43
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.53	0.43
2:B:2001:LAK:H18	2:B:2001:LAK:H7	1.99	0.43
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.54	0.43
1:B:390:SER:HA	1:B:391:HIS:HA	1.84	0.43
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.42
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.48	0.42
1:C:431:ARG:NH2	6:C:4487:HOH:O	2.52	0.42
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:LAK:H17	6:B:4098:HOH:O	2.18	0.42
1:B:358:GLU:HB3	1:B:367:MET:HG2	2.01	0.42
1:D:628:GLN:OE1	5:D:8002:DMS:C2	2.67	0.42
1:A:153:TRP:HB2	1:A:185:ALA:HB3	2.01	0.42
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.42
1:B:546:LEU:HA	6:B:4149:HOH:O	2.20	0.42
1:A:372:MET:HE1	1:A:395:HIS:HB3	2.01	0.42
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.55	0.42
1:B:147:ASN:HA	1:B:148:SER:HA	1.67	0.42
1:D:883:GLY:HA3	1:D:987:ASP:HA	2.02	0.42
1:A:372:MET:CE	1:A:395:HIS:HB3	2.49	0.41
1:A:793:ILE:HA	1:A:807:VAL:HG11	2.03	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41
1:A:942:ARG:HA	1:A:953:GLY:O	2.21	0.41
1:B:1023:LYS:HA	6:B:4592:HOH:O	2.18	0.41
1:D:524:LEU:HD11	1:D:562:LEU:HG	2.02	0.41
1:C:226:HIS:O	1:C:242:ALA:HA	2.21	0.41
1:D:251:ARG:HD3	1:D:253:TYR:OH	2.21	0.41
1:A:525:SER:O	1:B:561:ARG:HD3	2.21	0.41
1:B:614:HIS:HD1	1:B:929:TYR:HE2	1.69	0.41
1:C:225:PHE:HA	1:C:243:GLU:O	2.21	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.82	0.41
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.20	0.41
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.56	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.40
1:B:907:PRO:HG2	1:B:990:HIS:O	2.22	0.40
1:C:333:ARG:HA	1:C:345:ASN:OD1	2.21	0.40
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.56	0.40
1:C:358:GLU:HB3	1:C:367:MET:HG2	2.04	0.40
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.02	0.40
1:A:710:GLU:HG3	5:A:8015:DMS:H11	2.04	0.40
1:A:301:TRP:CH2	1:A:452:SER:HA	2.56	0.40
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.57	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%)	983 (97%)	30 (3%)	0	100	100
1	B	1013/1052 (96%)	981 (97%)	32 (3%)	0	100	100
1	C	1013/1052 (96%)	987 (97%)	26 (3%)	0	100	100
1	D	1013/1052 (96%)	981 (97%)	32 (3%)	0	100	100
All	All	4052/4208 (96%)	3932 (97%)	120 (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%)	859 (99%)	9 (1%)	82	91
1	B	868/898 (97%)	863 (99%)	5 (1%)	90	95
1	C	868/898 (97%)	860 (99%)	8 (1%)	84	92
1	D	868/898 (97%)	860 (99%)	8 (1%)	84	92
All	All	3472/3592 (97%)	3442 (99%)	30 (1%)	84	92

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	80	GLU

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Mol	Chain	Res	Type
1	A	230	ARG
1	A	245	GLN
1	A	333	ARG
1	A	546	LEU
1	A	672	VAL
1	A	687	GLN
1	A	956	GLN
1	B	333	ARG
1	B	344	LEU
1	B	546	LEU
1	B	687	GLN
1	B	956	GLN
1	C	237	ARG
1	C	333	ARG
1	C	344	LEU
1	C	546	LEU
1	C	672	VAL
1	C	774	LYS
1	C	956	GLN
1	C	1023	LYS
1	D	80	GLU
1	D	178	ARG
1	D	333	ARG
1	D	546	LEU
1	D	663	LEU
1	D	672	VAL
1	D	772	ASP
1	D	956	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	761	GLN
1	B	1022	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 26 are monoatomic - leaving 81 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$
2	LAK	A	2001	4	24,24,24	0.68	1 (4%)	35,35,35	1.82	8 (22%)
5	DMS	A	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.61	0
5	DMS	A	8002	-	3,3,3	2.54	1 (33%)	3,3,3	0.46	0
5	DMS	A	8003	-	3,3,3	2.58	1 (33%)	3,3,3	0.54	0
5	DMS	A	8004	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
5	DMS	A	8005	-	3,3,3	2.60	1 (33%)	3,3,3	0.40	0
5	DMS	A	8006	-	3,3,3	2.61	1 (33%)	3,3,3	0.49	0
5	DMS	A	8007	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
5	DMS	A	8008	-	3,3,3	2.58	1 (33%)	3,3,3	0.49	0
5	DMS	A	8009	-	3,3,3	2.57	1 (33%)	3,3,3	0.42	0
5	DMS	A	8010	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
5	DMS	A	8011	-	3,3,3	2.62	1 (33%)	3,3,3	0.44	0
5	DMS	A	8012	-	3,3,3	2.59	1 (33%)	3,3,3	0.40	0
5	DMS	A	8013	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
5	DMS	A	8014	-	3,3,3	2.61	1 (33%)	3,3,3	0.40	0
5	DMS	A	8015	-	3,3,3	2.58	1 (33%)	3,3,3	0.45	0
5	DMS	A	8016	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
5	DMS	A	8017	-	3,3,3	2.60	1 (33%)	3,3,3	0.51	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	2.63	1 (33%)	3,3,3	0.54	0
2	LAK	B	2001	4	24,24,24	0.75	1 (4%)	35,35,35	1.71	7 (20%)
5	DMS	B	8001	-	3,3,3	2.50	1 (33%)	3,3,3	0.42	0
5	DMS	B	8002	-	3,3,3	2.53	1 (33%)	3,3,3	0.39	0
5	DMS	B	8003	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
5	DMS	B	8004	-	3,3,3	2.57	1 (33%)	3,3,3	0.43	0
5	DMS	B	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.24	0
5	DMS	B	8006	-	3,3,3	2.60	1 (33%)	3,3,3	0.61	0
5	DMS	B	8007	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
5	DMS	B	8008	-	3,3,3	2.62	1 (33%)	3,3,3	0.35	0
5	DMS	B	8009	-	3,3,3	2.53	1 (33%)	3,3,3	0.28	0
5	DMS	B	8010	-	3,3,3	2.62	1 (33%)	3,3,3	0.53	0
5	DMS	B	8011	-	3,3,3	2.59	1 (33%)	3,3,3	0.56	0
5	DMS	B	8012	-	3,3,3	2.63	1 (33%)	3,3,3	0.52	0
5	DMS	B	8013	-	3,3,3	2.60	1 (33%)	3,3,3	0.45	0
5	DMS	B	8014	-	3,3,3	2.59	1 (33%)	3,3,3	0.40	0
5	DMS	B	8015	-	3,3,3	2.59	1 (33%)	3,3,3	0.38	0
5	DMS	B	8016	-	3,3,3	2.55	1 (33%)	3,3,3	0.54	0
5	DMS	B	8017	-	3,3,3	2.62	1 (33%)	3,3,3	0.45	0
5	DMS	B	8018	-	3,3,3	2.54	1 (33%)	3,3,3	0.38	0
5	DMS	B	8019	-	3,3,3	2.52	1 (33%)	3,3,3	0.39	0
5	DMS	B	8020	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
5	DMS	B	8021	-	3,3,3	2.56	1 (33%)	3,3,3	0.42	0
5	DMS	B	8022	-	3,3,3	2.58	1 (33%)	3,3,3	0.51	0
5	DMS	B	8023	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0
5	DMS	B	8024	-	3,3,3	2.41	1 (33%)	3,3,3	0.58	0
2	LAK	C	2001	4	24,24,24	0.66	1 (4%)	35,35,35	1.67	6 (17%)
5	DMS	C	8001	-	3,3,3	2.51	1 (33%)	3,3,3	0.54	0
5	DMS	C	8002	-	3,3,3	2.55	1 (33%)	3,3,3	0.35	0
5	DMS	C	8003	-	3,3,3	2.58	1 (33%)	3,3,3	0.33	0
5	DMS	C	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.50	0
5	DMS	C	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.39	0
5	DMS	C	8006	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
5	DMS	C	8007	-	3,3,3	2.62	1 (33%)	3,3,3	0.51	0
5	DMS	C	8008	-	3,3,3	2.53	1 (33%)	3,3,3	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8009	-	3,3,3	2.60	1 (33%)	3,3,3	0.46	0
5	DMS	C	8010	-	3,3,3	2.60	1 (33%)	3,3,3	0.57	0
5	DMS	C	8011	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
5	DMS	C	8012	-	3,3,3	2.60	1 (33%)	3,3,3	0.43	0
5	DMS	C	8013	-	3,3,3	2.58	1 (33%)	3,3,3	0.43	0
5	DMS	C	8014	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
5	DMS	C	8015	-	3,3,3	2.67	1 (33%)	3,3,3	0.44	0
5	DMS	C	8016	-	3,3,3	2.60	1 (33%)	3,3,3	0.49	0
5	DMS	C	8017	-	3,3,3	2.41	1 (33%)	3,3,3	0.33	0
5	DMS	C	8018	-	3,3,3	2.60	1 (33%)	3,3,3	0.43	0
5	DMS	C	8019	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
5	DMS	C	8020	-	3,3,3	2.39	1 (33%)	3,3,3	0.63	0
2	LAK	D	2001	4	24,24,24	0.68	1 (4%)	35,35,35	1.70	7 (20%)
5	DMS	D	8001	-	3,3,3	2.55	1 (33%)	3,3,3	0.53	0
5	DMS	D	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.52	0
5	DMS	D	8003	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
5	DMS	D	8004	-	3,3,3	2.60	1 (33%)	3,3,3	0.51	0
5	DMS	D	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.25	0
5	DMS	D	8006	-	3,3,3	2.59	1 (33%)	3,3,3	0.39	0
5	DMS	D	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
5	DMS	D	8008	-	3,3,3	2.59	1 (33%)	3,3,3	0.47	0
5	DMS	D	8009	-	3,3,3	2.58	1 (33%)	3,3,3	0.45	0
5	DMS	D	8010	-	3,3,3	2.61	1 (33%)	3,3,3	0.42	0
5	DMS	D	8011	-	3,3,3	2.60	1 (33%)	3,3,3	0.46	0
5	DMS	D	8012	-	3,3,3	2.60	1 (33%)	3,3,3	0.44	0
5	DMS	D	8013	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
5	DMS	D	8014	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
5	DMS	D	8015	-	3,3,3	2.60	1 (33%)	3,3,3	0.61	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	LAK	A	2001	4	-	0/7/47/47	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	A	8001	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8002	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8003	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8004	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8005	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8006	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8007	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8008	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8009	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8010	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8011	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8012	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8013	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8014	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8015	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8016	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8017	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8018	-	-	0/0/0/0	0/0/0/0
2	LAK	B	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	B	8001	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8002	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8003	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8004	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8005	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8006	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8007	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8008	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8009	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8010	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8011	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8012	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8013	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8014	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8015	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8016	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8017	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8018	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8019	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8020	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8021	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8022	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8023	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8024	-	-	0/0/0/0	0/0/0/0
2	LAK	C	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	C	8001	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8002	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8003	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8004	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8005	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8006	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8007	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8008	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8009	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8010	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8011	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8012	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8013	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8014	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8015	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8016	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8017	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8018	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8019	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8020	-	-	0/0/0/0	0/0/0/0
2	LAK	D	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	D	8001	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8002	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8003	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8004	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8005	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8006	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8007	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8008	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8009	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8010	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8011	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8012	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8013	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8014	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8015	-	-	0/0/0/0	0/0/0/0

All (81) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	LAK	O1-C1	2.15	1.44	1.40
2	A	2001	LAK	O1-C1	2.18	1.44	1.40
2	C	2001	LAK	O1-C1	2.37	1.44	1.40
2	B	2001	LAK	O1-C1	2.64	1.44	1.40
5	C	8020	DMS	O-S	4.03	1.77	1.50
5	B	8024	DMS	O-S	4.05	1.78	1.50
5	C	8017	DMS	O-S	4.06	1.78	1.50
5	B	8001	DMS	O-S	4.19	1.79	1.50
5	C	8001	DMS	O-S	4.21	1.79	1.50
5	B	8019	DMS	O-S	4.23	1.79	1.50
5	B	8018	DMS	O-S	4.24	1.79	1.50
5	C	8008	DMS	O-S	4.24	1.79	1.50
5	B	8002	DMS	O-S	4.25	1.79	1.50
5	B	8009	DMS	O-S	4.26	1.79	1.50
5	D	8001	DMS	O-S	4.26	1.79	1.50
5	A	8002	DMS	O-S	4.27	1.79	1.50
5	A	8001	DMS	O-S	4.29	1.79	1.50
5	B	8016	DMS	O-S	4.30	1.79	1.50
5	C	8002	DMS	O-S	4.30	1.79	1.50
5	A	8009	DMS	O-S	4.30	1.79	1.50
5	A	8008	DMS	O-S	4.31	1.79	1.50
5	B	8004	DMS	O-S	4.31	1.79	1.50
5	B	8021	DMS	O-S	4.32	1.79	1.50
5	B	8011	DMS	O-S	4.32	1.79	1.50
5	D	8009	DMS	O-S	4.32	1.79	1.50
5	B	8005	DMS	O-S	4.33	1.80	1.50
5	B	8022	DMS	O-S	4.33	1.80	1.50
5	A	8012	DMS	O-S	4.33	1.80	1.50
5	C	8013	DMS	O-S	4.33	1.80	1.50
5	C	8010	DMS	O-S	4.34	1.80	1.50
5	A	8003	DMS	O-S	4.34	1.80	1.50
5	A	8015	DMS	O-S	4.34	1.80	1.50
5	C	8005	DMS	O-S	4.34	1.80	1.50
5	D	8008	DMS	O-S	4.35	1.80	1.50
5	D	8006	DMS	O-S	4.35	1.80	1.50
5	C	8003	DMS	O-S	4.35	1.80	1.50
5	D	8005	DMS	O-S	4.35	1.80	1.50
5	B	8014	DMS	O-S	4.35	1.80	1.50
5	D	8014	DMS	O-S	4.35	1.80	1.50
5	C	8012	DMS	O-S	4.35	1.80	1.50
5	D	8011	DMS	O-S	4.35	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8015	DMS	O-S	4.35	1.80	1.50
5	C	8009	DMS	O-S	4.36	1.80	1.50
5	B	8015	DMS	O-S	4.36	1.80	1.50
5	A	8017	DMS	O-S	4.36	1.80	1.50
5	B	8006	DMS	O-S	4.36	1.80	1.50
5	C	8011	DMS	O-S	4.37	1.80	1.50
5	C	8018	DMS	O-S	4.37	1.80	1.50
5	D	8010	DMS	O-S	4.37	1.80	1.50
5	B	8013	DMS	O-S	4.37	1.80	1.50
5	A	8014	DMS	O-S	4.37	1.80	1.50
5	D	8004	DMS	O-S	4.37	1.80	1.50
5	B	8010	DMS	O-S	4.37	1.80	1.50
5	A	8005	DMS	O-S	4.37	1.80	1.50
5	C	8004	DMS	O-S	4.38	1.80	1.50
5	C	8016	DMS	O-S	4.38	1.80	1.50
5	A	8016	DMS	O-S	4.38	1.80	1.50
5	C	8007	DMS	O-S	4.38	1.80	1.50
5	A	8006	DMS	O-S	4.38	1.80	1.50
5	C	8019	DMS	O-S	4.39	1.80	1.50
5	D	8012	DMS	O-S	4.39	1.80	1.50
5	B	8023	DMS	O-S	4.39	1.80	1.50
5	A	8011	DMS	O-S	4.40	1.80	1.50
5	B	8008	DMS	O-S	4.40	1.80	1.50
5	A	8018	DMS	O-S	4.40	1.80	1.50
5	D	8003	DMS	O-S	4.40	1.80	1.50
5	B	8012	DMS	O-S	4.41	1.80	1.50
5	D	8007	DMS	O-S	4.41	1.80	1.50
5	A	8013	DMS	O-S	4.41	1.80	1.50
5	B	8020	DMS	O-S	4.41	1.80	1.50
5	D	8002	DMS	O-S	4.41	1.80	1.50
5	B	8017	DMS	O-S	4.41	1.80	1.50
5	B	8003	DMS	O-S	4.41	1.80	1.50
5	A	8004	DMS	O-S	4.42	1.80	1.50
5	A	8010	DMS	O-S	4.42	1.80	1.50
5	C	8014	DMS	O-S	4.42	1.80	1.50
5	D	8013	DMS	O-S	4.42	1.80	1.50
5	A	8007	DMS	O-S	4.43	1.80	1.50
5	C	8015	DMS	O-S	4.47	1.80	1.50
5	C	8006	DMS	O-S	4.47	1.81	1.50
5	B	8007	DMS	O-S	4.51	1.81	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2001	LAK	C2'-C3'-C4'	2.04	114.60	110.79
2	B	2001	LAK	O5-C5-C4	2.17	113.76	109.68
2	B	2001	LAK	C3'-C4'-C5'	2.38	114.35	110.20
2	A	2001	LAK	C1'-C2'-C3'	2.54	114.20	110.43
2	B	2001	LAK	O5-C1-C2	2.56	115.53	110.28
2	C	2001	LAK	C3'-C4'-C5'	2.57	114.67	110.20
2	C	2001	LAK	O5-C5-C4	2.61	114.57	109.68
2	A	2001	LAK	O5-C5-C4	2.77	114.88	109.68
2	D	2001	LAK	C1'-C2'-C3'	2.83	114.63	110.43
2	D	2001	LAK	O5-C5-C4	2.90	115.13	109.68
2	A	2001	LAK	C2'-C3'-C4'	2.96	116.31	110.79
2	D	2001	LAK	C2'-C3'-C4'	2.96	116.32	110.79
2	D	2001	LAK	O5-C1-C2	3.00	116.42	110.28
2	C	2001	LAK	O1-C6'-C5'	3.09	114.69	109.08
2	C	2001	LAK	O5-C1-C2	3.10	116.64	110.28
2	D	2001	LAK	O1-C1-C2	3.22	112.11	108.04
2	A	2001	LAK	O1-C6'-C5'	3.24	114.95	109.08
2	D	2001	LAK	C3'-C4'-C5'	3.30	115.95	110.20
2	A	2001	LAK	O5-C1-C2	3.36	117.17	110.28
2	A	2001	LAK	O1-C1-C2	3.41	112.34	108.04
2	B	2001	LAK	O1-C6'-C5'	3.64	115.68	109.08
2	A	2001	LAK	C3'-C4'-C5'	4.11	117.36	110.20
2	C	2001	LAK	O1-C1-C2	4.18	113.32	108.04
2	B	2001	LAK	O1-C1-C2	4.27	113.44	108.04
2	A	2001	LAK	C1-O5-C5	5.36	124.15	113.75
2	D	2001	LAK	C1-O5-C5	5.37	124.16	113.75
2	C	2001	LAK	C1-O5-C5	5.70	124.81	113.75
2	B	2001	LAK	C1-O5-C5	5.76	124.92	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8015	DMS	1	0
2	B	2001	LAK	2	0
5	C	8013	DMS	1	0
2	D	2001	LAK	1	0
5	D	8002	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, 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%)	-0.39	28 (2%) 56 55	21, 35, 61, 98	0
1	B	1015/1052 (96%)	-0.46	26 (2%) 59 58	20, 30, 58, 97	0
1	C	1015/1052 (96%)	-0.49	26 (2%) 59 58	19, 30, 55, 96	0
1	D	1015/1052 (96%)	-0.35	28 (2%) 56 55	23, 36, 60, 106	0
All	All	4060/4208 (96%)	-0.42	108 (2%) 58 57	19, 33, 59, 106	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	6.3
1	D	735	HIS	6.2
1	B	689	GLU	6.0
1	D	689	GLU	5.7
1	A	689	GLU	5.6
1	B	731	PRO	5.5
1	A	733	ALA	5.5
1	A	799	THR	5.4
1	A	9	VAL	5.1
1	A	732	ALA	5.0
1	B	799	THR	4.9
1	B	733	ALA	4.9
1	B	12	GLN	4.8
1	A	730	LEU	4.7
1	C	731	PRO	4.6
1	B	1023	LYS	4.6
1	D	731	PRO	4.6
1	C	689	GLU	4.5
1	D	732	ALA	4.4
1	A	1023	LYS	4.3
1	C	686	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	4.3
1	D	730	LEU	4.2
1	C	1023	LYS	4.0
1	B	732	ALA	4.0
1	B	684	GLU	4.0
1	A	12	GLN	3.9
1	D	10	VAL	3.8
1	C	732	ALA	3.6
1	D	687	GLN	3.6
1	D	799	THR	3.6
1	D	79	PRO	3.6
1	C	580	GLU	3.4
1	A	684	GLU	3.4
1	A	686	PRO	3.4
1	A	580	GLU	3.3
1	D	729	THR	3.3
1	D	11	LEU	3.3
1	D	801	ILE	3.3
1	C	11	LEU	3.2
1	C	733	ALA	3.2
1	B	770	ILE	3.2
1	C	1022	GLN	3.2
1	D	733	ALA	3.2
1	D	684	GLU	3.2
1	C	9	VAL	3.1
1	D	772	ASP	3.1
1	D	179	ALA	3.1
1	D	12	GLN	3.1
1	B	735	HIS	3.1
1	D	580	GLU	3.1
1	B	686	PRO	3.0
1	B	80	GLU	3.0
1	A	687	GLN	3.0
1	C	12	GLN	3.0
1	C	772	ASP	3.0
1	A	179	ALA	2.9
1	D	582	GLY	2.9
1	B	10	VAL	2.9
1	A	595	THR	2.9
1	C	684	GLU	2.9
1	C	735	HIS	2.9
1	D	186	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	687	GLN	2.9
1	C	831	ALA	2.8
1	A	685	LEU	2.8
1	D	581	ASN	2.8
1	A	734	SER	2.7
1	A	131	GLU	2.7
1	C	10	VAL	2.7
1	D	130	ASP	2.6
1	D	131	GLU	2.6
1	A	71	GLU	2.6
1	A	800	ARG	2.6
1	C	799	THR	2.6
1	C	800	ARG	2.6
1	C	685	LEU	2.5
1	D	1023	LYS	2.5
1	C	730	LEU	2.5
1	B	730	LEU	2.5
1	D	686	PRO	2.5
1	B	831	ALA	2.4
1	A	11	LEU	2.4
1	B	685	LEU	2.4
1	C	581	ASN	2.4
1	B	9	VAL	2.4
1	B	186	VAL	2.4
1	B	772	ASP	2.4
1	A	79	PRO	2.4
1	A	729	THR	2.4
1	A	80	GLU	2.3
1	B	11	LEU	2.3
1	A	582	GLY	2.3
1	C	832	ASP	2.3
1	C	773	LYS	2.2
1	B	773	LYS	2.2
1	D	800	ARG	2.1
1	A	845	GLN	2.1
1	D	845	GLN	2.1
1	A	188	VAL	2.1
1	B	1022	GLN	2.1
1	D	798	ALA	2.1
1	C	819	GLU	2.0
1	C	582	GLY	2.0
1	B	832	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	739	HIS	2.0
1	B	729	THR	2.0
1	B	800	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	DMS	A	8018	4/4	0.74	0.20	12.73	83,83,85,87	0
5	DMS	C	8004	4/4	0.90	0.19	11.70	57,61,62,63	0
5	DMS	B	8013	4/4	0.90	0.19	9.71	73,73,74,77	0
5	DMS	A	8017	4/4	0.83	0.28	8.70	64,70,73,74	0
5	DMS	B	8016	4/4	0.93	0.15	7.59	62,64,65,70	0
5	DMS	A	8014	4/4	0.91	0.19	6.80	70,72,74,74	0
5	DMS	C	8020	4/4	0.96	0.13	6.35	51,55,55,57	0
5	DMS	C	8015	4/4	0.94	0.12	5.69	57,57,58,62	0
5	DMS	B	8023	4/4	0.89	0.13	5.66	72,73,74,75	0
3	MG	D	3002	1/1	0.97	0.19	5.61	35,35,35,35	0
4	NA	C	3101	1/1	0.98	0.15	5.37	27,27,27,27	0
5	DMS	B	8004	4/4	0.93	0.16	5.13	43,44,49,52	0
5	DMS	C	8013	4/4	0.95	0.15	4.30	67,69,69,72	0
5	DMS	A	8003	4/4	0.95	0.16	4.21	40,49,52,53	0
5	DMS	D	8004	4/4	0.90	0.17	4.01	56,58,59,61	0
5	DMS	B	8021	4/4	0.96	0.13	3.98	41,42,43,46	0
5	DMS	A	8004	4/4	0.93	0.13	3.67	56,57,63,64	0
5	DMS	A	8006	4/4	0.95	0.16	3.32	68,69,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8015	4/4	0.96	0.25	3.01	71,72,72,72	0
5	DMS	B	8005	4/4	0.98	0.16	2.90	44,48,51,53	0
5	DMS	C	8003	4/4	0.99	0.17	2.75	44,47,47,47	0
4	NA	B	3103	1/1	0.88	0.20	2.68	46,46,46,46	0
2	LAK	C	2001	23/23	0.93	0.14	2.56	25,35,67,68	0
5	DMS	D	8015	4/4	0.93	0.24	2.53	69,71,71,71	0
2	LAK	D	2001	23/23	0.90	0.14	2.49	30,42,68,70	0
5	DMS	D	8002	4/4	0.97	0.13	2.44	33,33,36,44	0
5	DMS	B	8006	4/4	0.85	0.20	2.35	57,63,65,67	0
5	DMS	C	8016	4/4	0.91	0.16	2.18	64,64,65,67	0
5	DMS	B	8019	4/4	0.89	0.20	2.07	68,71,71,71	0
2	LAK	A	2001	23/23	0.90	0.15	2.07	30,44,75,78	0
5	DMS	D	8012	4/4	0.87	0.19	2.02	59,60,63,65	0
5	DMS	D	8003	4/4	0.98	0.12	1.97	54,55,56,56	0
5	DMS	A	8005	4/4	0.98	0.16	1.90	46,47,50,51	0
5	DMS	A	8016	4/4	0.94	0.19	1.81	61,63,63,70	0
5	DMS	A	8013	4/4	0.84	0.20	1.75	75,78,79,84	0
5	DMS	B	8001	4/4	0.99	0.15	1.70	37,38,39,41	0
5	DMS	B	8020	4/4	0.94	0.17	1.66	71,72,72,72	0
5	DMS	B	8008	4/4	0.82	0.26	1.58	74,74,76,76	0
4	NA	A	3104	1/1	0.91	0.14	1.53	50,50,50,50	0
5	DMS	C	8002	4/4	0.97	0.10	1.50	31,34,40,42	0
5	DMS	A	8008	4/4	0.97	0.14	1.48	56,59,60,60	0
5	DMS	C	8019	4/4	0.97	0.11	1.41	53,53,57,61	0
5	DMS	D	8014	4/4	0.95	0.20	1.36	72,73,73,75	0
5	DMS	D	8006	4/4	0.89	0.19	1.31	74,77,79,80	0
5	DMS	A	8010	4/4	0.89	0.16	1.26	65,69,70,71	0
5	DMS	D	8001	4/4	0.98	0.13	1.25	39,40,41,42	0
5	DMS	B	8010	4/4	0.97	0.18	1.24	51,52,53,55	0
5	DMS	C	8001	4/4	0.98	0.12	1.23	33,36,37,40	0
5	DMS	C	8005	4/4	0.98	0.12	1.20	39,44,45,46	0
4	NA	D	3104	1/1	0.82	0.14	1.15	58,58,58,58	0
4	NA	C	3103	1/1	0.95	0.14	1.12	43,43,43,43	0
4	NA	B	3104	1/1	0.74	0.14	1.07	55,55,55,55	0
5	DMS	C	8017	4/4	0.96	0.14	0.96	65,66,66,69	0
5	DMS	D	8005	4/4	0.96	0.12	0.92	45,45,48,48	0
5	DMS	B	8015	4/4	0.87	0.19	0.88	81,81,82,83	0
5	DMS	C	8009	4/4	0.98	0.14	0.62	54,57,58,60	0
5	DMS	B	8003	4/4	0.98	0.13	0.61	44,49,49,49	0
5	DMS	B	8002	4/4	0.97	0.10	0.56	38,40,42,42	0
2	LAK	B	2001	23/23	0.93	0.13	0.54	25,38,62,69	0
4	NA	C	3104	1/1	0.84	0.12	0.51	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	C	8018	4/4	0.96	0.14	0.48	68,71,71,71	0
5	DMS	B	8009	4/4	0.98	0.14	0.39	49,53,55,55	0
5	DMS	A	8001	4/4	0.98	0.11	0.38	33,35,38,39	0
5	DMS	A	8009	4/4	0.94	0.16	0.38	56,61,63,64	0
5	DMS	D	8009	4/4	0.97	0.15	0.29	52,54,57,58	0
4	NA	A	3103	1/1	0.85	0.11	0.23	49,49,49,49	0
5	DMS	C	8008	4/4	0.98	0.10	0.21	39,39,41,42	0
5	DMS	A	8002	4/4	0.98	0.08	-0.30	43,44,45,47	0
5	DMS	B	8022	4/4	0.98	0.09	-0.34	51,53,54,55	0
4	NA	B	3102	1/1	0.96	0.07	-0.90	31,31,31,31	0
4	NA	A	3101	1/1	0.92	0.09	-1.08	34,34,34,34	0
4	NA	C	3102	1/1	0.96	0.06	-1.14	31,31,31,31	0
4	NA	D	3102	1/1	0.97	0.06	-1.16	33,33,33,33	0
3	MG	B	3001	1/1	0.99	0.09	-1.21	24,24,24,24	0
4	NA	A	3102	1/1	0.99	0.07	-1.26	30,30,30,30	0
3	MG	B	3002	1/1	0.96	0.07	-1.59	29,29,29,29	0
3	MG	D	3001	1/1	0.96	0.06	-1.64	32,32,32,32	0
4	NA	D	3103	1/1	0.92	0.07	-1.65	45,45,45,45	0
4	NA	B	3101	1/1	0.98	0.08	-1.77	27,27,27,27	0
4	NA	D	3101	1/1	0.97	0.08	-1.93	32,32,32,32	0
3	MG	A	3002	1/1	0.95	0.06	-2.36	39,39,39,39	0
3	MG	C	3002	1/1	0.98	0.04	-2.47	25,25,25,25	0
3	MG	C	3001	1/1	0.99	0.05	-3.47	22,22,22,22	0
3	MG	A	3001	1/1	0.99	0.04	-3.69	30,30,30,30	0
5	DMS	D	8011	4/4	0.94	0.23	-	64,67,69,72	0
3	MG	A	3006	1/1	0.88	0.07	-	67,67,67,67	0
5	DMS	D	8007	4/4	0.87	0.17	-	69,70,70,71	0
5	DMS	B	8007	4/4	0.92	0.14	-	47,49,55,57	0
5	DMS	C	8007	4/4	0.92	0.16	-	65,69,70,73	0
5	DMS	B	8011	4/4	0.91	0.27	-	58,61,64,65	0
5	DMS	C	8006	4/4	0.94	0.13	-	53,56,56,57	0
5	DMS	C	8011	4/4	0.92	0.17	-	52,58,58,61	0
5	DMS	B	8012	4/4	0.95	0.24	-	73,74,74,76	0
5	DMS	B	8024	4/4	0.97	0.10	-	60,60,61,62	0
5	DMS	C	8014	4/4	0.89	0.20	-	81,82,82,83	0
5	DMS	D	8008	4/4	0.98	0.11	-	56,59,60,61	0
5	DMS	A	8012	4/4	0.94	0.22	-	73,75,77,78	0
5	DMS	C	8012	4/4	0.95	0.20	-	70,70,72,72	0
5	DMS	A	8007	4/4	0.88	0.17	-	72,73,75,77	0
3	MG	B	3006	1/1	0.94	0.20	-	56,56,56,56	0
5	DMS	D	8013	4/4	0.73	0.28	-	72,74,78,79	0
5	DMS	B	8014	4/4	0.94	0.23	-	68,69,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8011	4/4	0.85	0.19	-	78,79,79,81	0
5	DMS	B	8017	4/4	0.94	0.14	-	72,73,74,75	0
5	DMS	D	8010	4/4	0.94	0.35	-	82,82,85,85	0
5	DMS	B	8018	4/4	0.88	0.19	-	69,71,72,74	0
5	DMS	C	8010	4/4	0.94	0.17	-	53,55,57,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.