



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:20 PM UTC

PDB ID : 3T2Q / pdb_00003t2q
Title : E. coli (lacZ) beta-galactosidase (S796D) in complex with galactonolactone
Authors : Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.
Deposited on : 2011-07-22
Resolution : 2.40 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

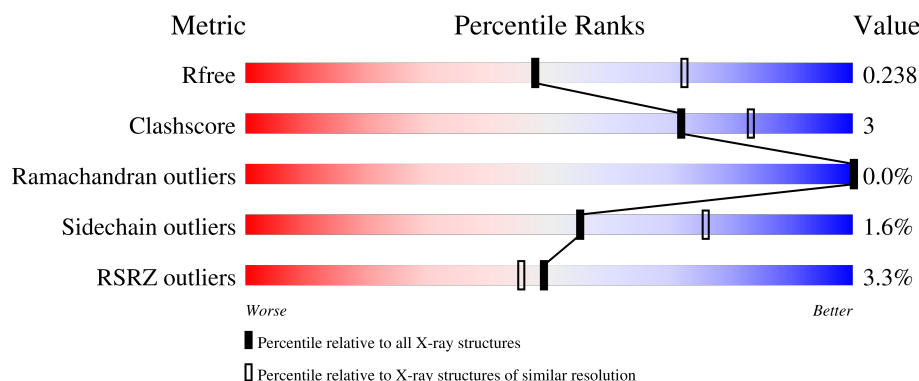
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	B	1052	
1	C	1052	
1	D	1052	

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	8003	-	-	X	-
5	DMS	C	8001	-	-	X	-
5	DMS	D	8003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35053 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	55	0	0
			8159	5160	1445	1516	38			
1	B	1015	Total	C	N	O	S	67	0	0
			8159	5160	1445	1516	38			
1	C	1015	Total	C	N	O	S	67	0	0
			8159	5160	1445	1516	38			
1	D	1015	Total	C	N	O	S	67	0	0
			8159	5160	1445	1516	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	ASP	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	ASP	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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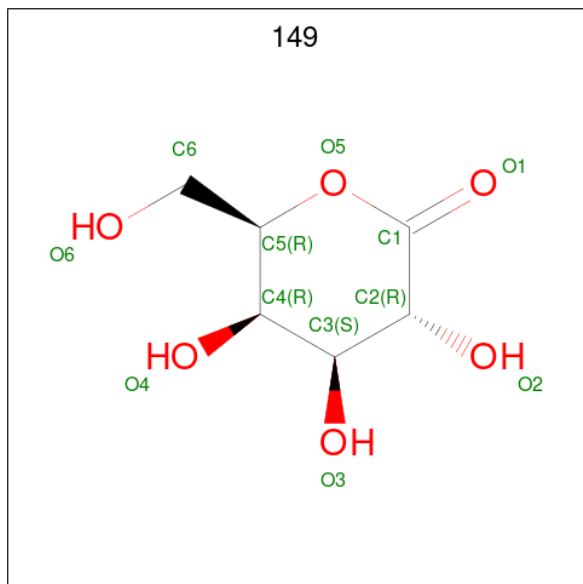
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	796	ASP	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	ASP	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	2	Total Mg 2 2	0	0

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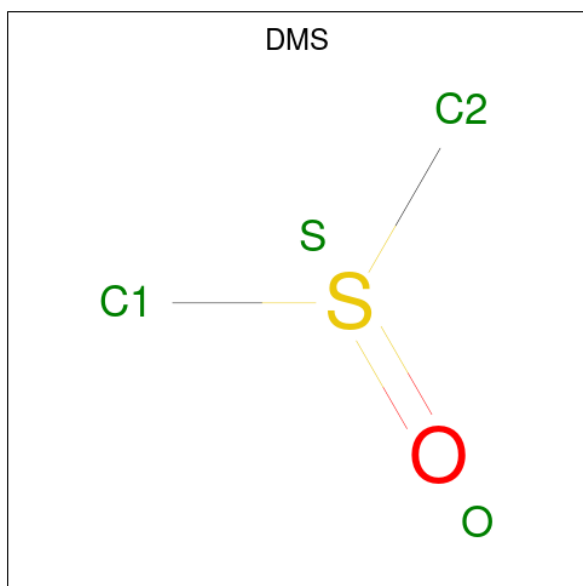
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

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

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

- 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	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	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	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

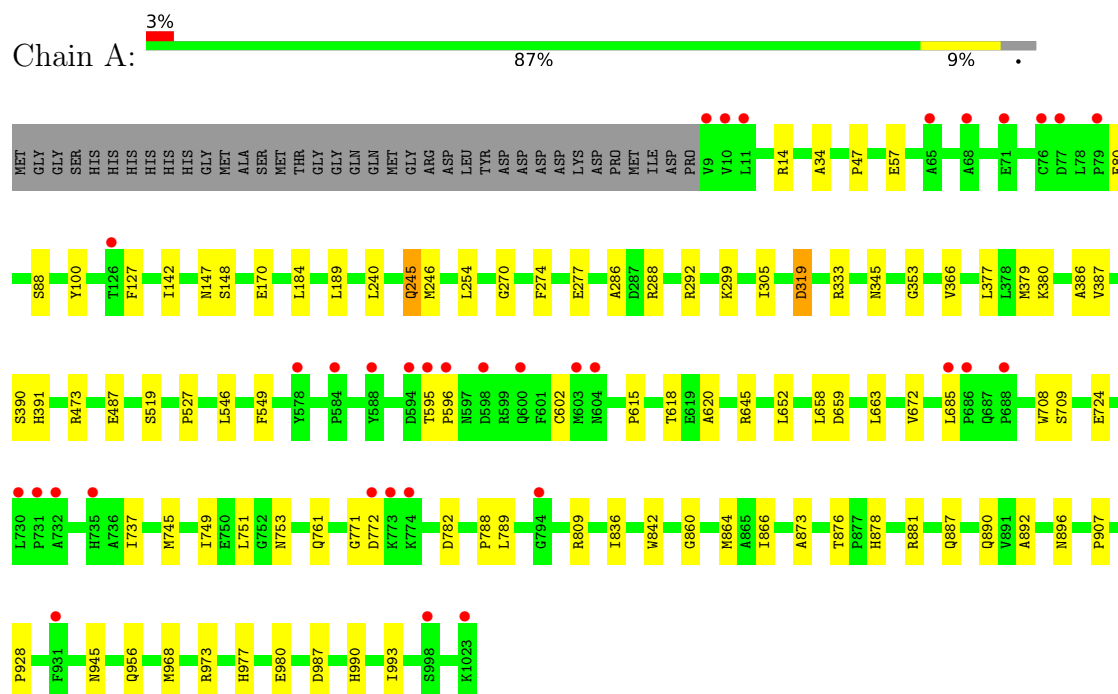
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	567	Total 567	O 567	0	0
6	B	565	Total 565	O 565	0	0
6	C	557	Total 557	O 557	0	0
6	D	465	Total 465	O 465	0	0

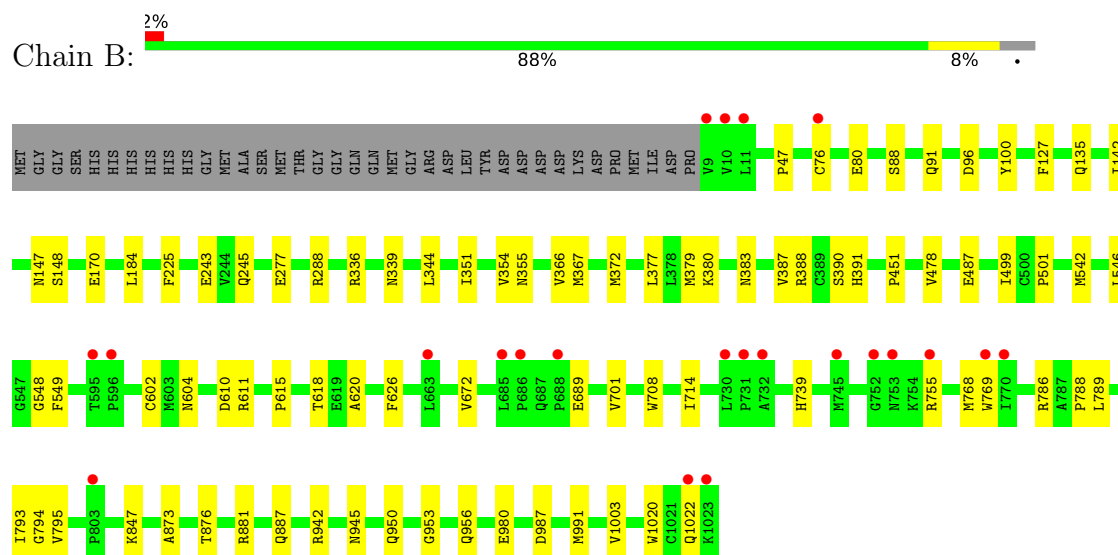
3 Residue-property plots [i](#)

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.

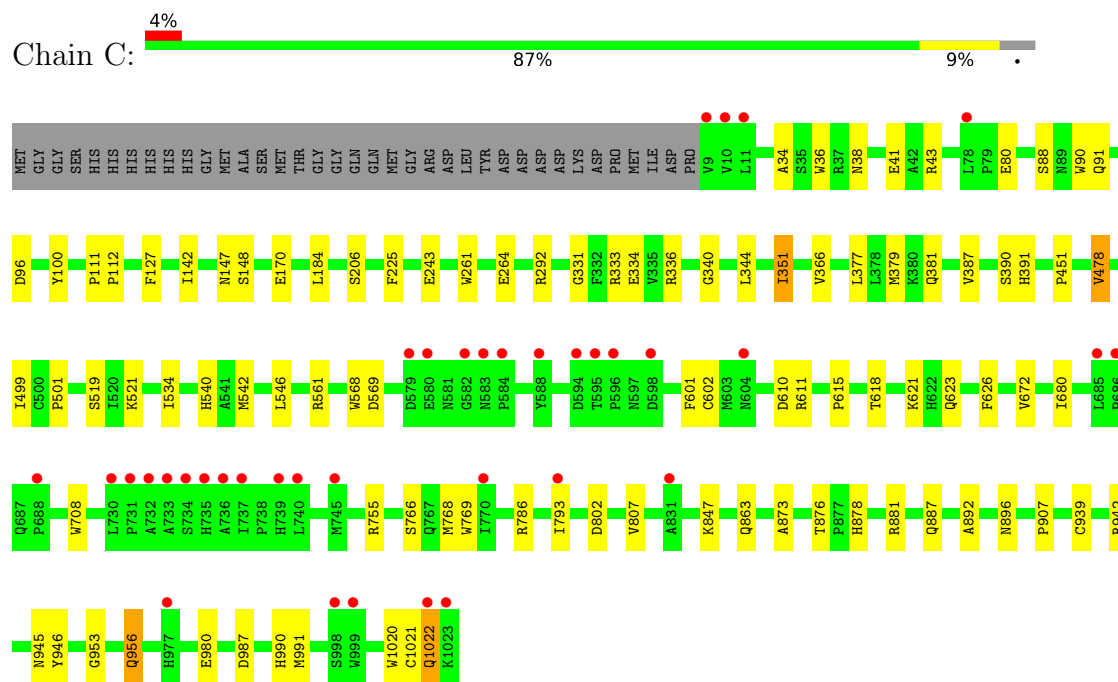
• Molecule 1: Beta-galactosidase



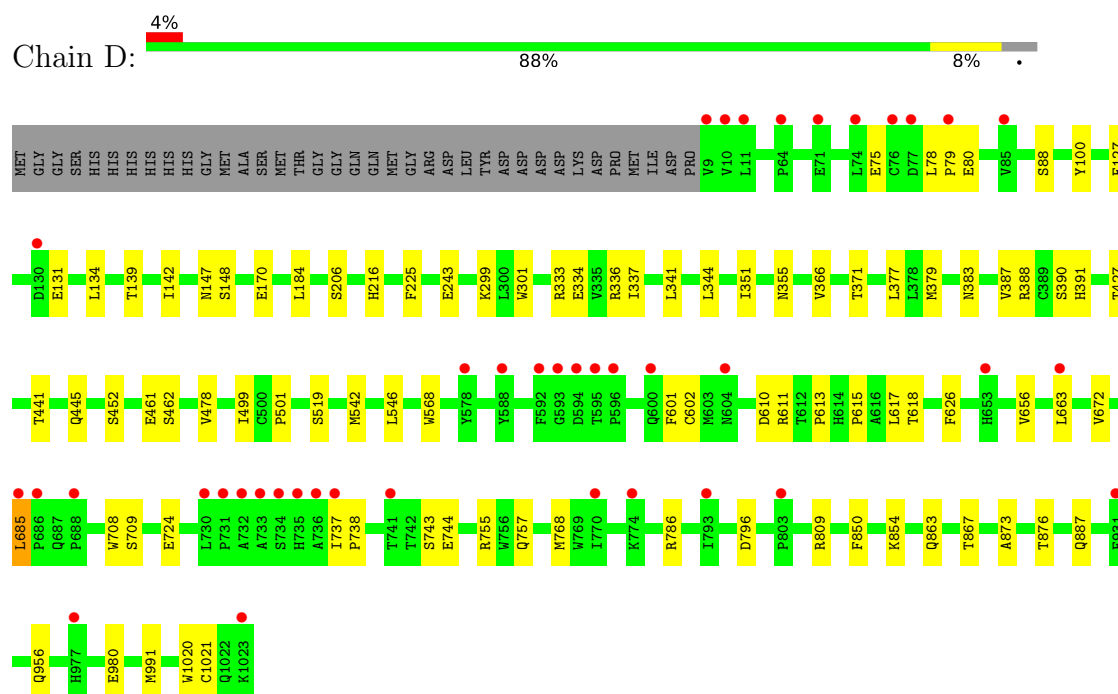
• Molecule 1: Beta-galactosidase



- 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	152.27Å 163.54Å 203.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.40 80.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.00-2.40) 98.9 (80.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.180 , 0.239 0.181 , 0.238	Depositor DCC
R_{free} test set	2829 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35053	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 41.79 % 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 2.2409e-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, 149, NA, DMS

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	0.54	0/8401	0.74	0/11461
1	B	0.54	0/8401	0.75	0/11461
1	C	0.54	0/8401	0.75	2/11461 (0.0%)
1	D	0.52	0/8401	0.75	0/11461
All	All	0.54	0/33604	0.75	2/45844 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	802	ASP	CA-C-N	5.90	125.60	119.64
1	C	802	ASP	C-N-CA	5.90	125.60	119.64

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	8159	0	7752	59	0
1	B	8159	0	7752	48	0
1	C	8159	0	7752	60	0
1	D	8159	0	7752	45	0
2	A	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	9	0	0
2	C	12	0	9	3	0
2	D	12	0	9	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
5	A	52	0	78	9	0
5	B	60	0	90	11	0
5	C	48	0	72	13	0
5	D	36	0	54	5	0
6	A	567	0	0	11	0
6	B	565	0	0	5	0
6	C	557	0	0	4	0
6	D	465	0	0	4	0
All	All	35053	0	31338	213	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 3.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.61	0.81
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.62	0.81
1:B:379:MET:HE1	1:B:387:VAL:HB	1.68	0.76
1:A:270:GLY:HA3	5:A:8005:DMS:H13	1.68	0.76
1:D:887:GLN:NE2	1:D:980:GLU:O	2.21	0.73
1:D:131:GLU:HA	1:D:134:LEU:HD12	1.72	0.71
1:C:336:ARG:HB3	5:C:8008:DMS:H23	1.73	0.71
1:B:887:GLN:NE2	1:B:980:GLU:O	2.25	0.70
1:C:379:MET:HE1	1:C:387:VAL:HB	1.73	0.69
1:C:540:HIS:HE2	2:C:2001:149:C6	2.06	0.69
5:C:8003:DMS:H13	6:C:4066:HOH:O	1.92	0.68
1:A:246:MET:CE	1:A:254:LEU:HD13	2.24	0.67
1:C:542:MET:HE3	1:C:601:PHE:HA	1.76	0.66
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:HIS:HB3	6:A:4480:HOH:O	1.95	0.65
1:B:991:MET:HE3	1:B:1003:VAL:HG21	1.78	0.64
1:C:331:GLY:O	5:C:8001:DMS:H13	1.97	0.63
1:C:615:PRO:O	1:C:618:THR:HG22	1.98	0.63
1:A:246:MET:HE1	1:A:254:LEU:HD13	1.80	0.62
1:A:245:GLN:HG3	1:A:288:ARG:HG2	1.80	0.62
1:B:615:PRO:O	1:B:618:THR:HG22	2.00	0.62
1:A:246:MET:HE1	1:A:254:LEU:CD1	2.30	0.61
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.35	0.61
1:A:379:MET:HE1	1:A:387:VAL:HB	1.81	0.61
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.35	0.60
1:D:379:MET:HE1	1:D:387:VAL:HB	1.83	0.60
1:B:945:ASN:OD1	1:B:950:GLN:HG3	2.02	0.60
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.37	0.59
1:B:755:ARG:HB3	1:B:769:TRP:HB2	1.83	0.59
1:D:127:PHE:HE1	1:D:184:LEU:HG	1.67	0.59
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.38	0.59
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.38	0.59
1:A:380:LYS:O	5:A:8003:DMS:H11	2.03	0.59
1:B:383:ASN:HA	5:B:8003:DMS:H12	1.85	0.58
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.86	0.58
1:B:701:VAL:HG22	1:B:714:ILE:HD13	1.85	0.58
1:C:88:SER:HA	1:C:366:VAL:HG21	1.86	0.58
1:A:270:GLY:CA	5:A:8005:DMS:H13	2.32	0.58
1:B:873:ALA:O	1:B:876:THR:HG22	2.03	0.58
1:A:887:GLN:NE2	1:A:980:GLU:O	2.36	0.57
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.40	0.57
1:B:336:ARG:HB3	5:B:8008:DMS:H23	1.87	0.57
1:B:739:HIS:HB2	6:B:4447:HOH:O	2.05	0.57
1:C:38:ASN:HB3	1:C:41:GLU:HG3	1.87	0.56
1:D:333:ARG:NH1	5:D:8001:DMS:H12	2.19	0.56
1:A:724:GLU:O	1:B:847:LYS:NZ	2.36	0.56
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.70	0.56
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.40	0.56
1:D:615:PRO:O	1:D:618:THR:HG22	2.05	0.56
1:B:380:LYS:O	5:B:8003:DMS:H11	2.06	0.55
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.37	0.55
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.42	0.55
1:C:878:HIS:HD2	6:C:4063:HOH:O	1.89	0.55
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.42	0.55
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ALA:O	1:A:876:THR:HG22	2.07	0.54
1:D:757:GLN:NE2	6:D:4307:HOH:O	2.39	0.54
1:A:615:PRO:O	1:A:618:THR:HG22	2.08	0.54
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.90	0.54
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.43	0.54
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.90	0.54
1:B:451:PRO:HA	5:B:8001:DMS:H23	1.90	0.54
1:C:793:ILE:HD13	1:C:807:VAL:HG11	1.90	0.53
1:D:744:GLU:HG2	6:D:4023:HOH:O	2.09	0.53
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.91	0.53
1:C:873:ALA:O	1:C:876:THR:HG22	2.09	0.53
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.90	0.53
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.90	0.52
1:C:847:LYS:NZ	1:D:724:GLU:O	2.43	0.52
1:A:809:ARG:HD2	6:A:4466:HOH:O	2.10	0.52
1:B:367:MET:HB3	1:B:372:MET:HE2	1.92	0.51
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.92	0.51
1:A:270:GLY:HA3	5:A:8005:DMS:C1	2.40	0.51
1:A:47:PRO:HA	5:A:8009:DMS:H12	1.92	0.51
1:B:47:PRO:HA	5:B:8013:DMS:H12	1.91	0.51
1:B:626:PHE:HE1	5:B:8003:DMS:H12	1.75	0.51
1:C:626:PHE:HE1	5:C:8003:DMS:H12	1.76	0.51
1:C:540:HIS:HE2	2:C:2001:149:H61	1.76	0.50
1:A:57:GLU:O	5:A:8010:DMS:H12	2.11	0.50
1:C:626:PHE:CE1	5:C:8003:DMS:H12	2.46	0.50
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.75	0.50
1:D:441:THR:O	1:D:445:GLN:HG3	2.11	0.50
1:D:809:ARG:HD2	6:D:4271:HOH:O	2.11	0.50
1:B:225:PHE:HA	1:B:243:GLU:O	2.12	0.50
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.46	0.50
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.12	0.50
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:B:788:PRO:HB2	1:B:793:ILE:HD11	1.94	0.49
1:C:36:TRP:HH2	5:C:8004:DMS:H23	1.77	0.49
1:C:610:ASP:O	1:C:611:ARG:HB2	2.12	0.49
5:A:8003:DMS:H13	6:A:4050:HOH:O	2.12	0.49
5:D:8003:DMS:H13	6:D:4077:HOH:O	2.12	0.49
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.12	0.49
1:D:873:ALA:O	1:D:876:THR:HG22	2.13	0.49
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.95	0.49
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:ARG:HB3	1:C:769:TRP:HB2	1.94	0.49
1:D:427:THR:HG21	1:D:462:SER:HB3	1.95	0.49
1:A:864:MET:HE3	1:A:866:ILE:HD11	1.95	0.49
1:C:292:ARG:HH12	5:C:8009:DMS:H23	1.78	0.49
1:D:542:MET:HE3	1:D:601:PHE:HA	1.94	0.48
1:A:761:GLN:HB2	6:A:4431:HOH:O	2.11	0.48
1:A:277:GLU:HG2	6:A:4305:HOH:O	2.12	0.48
1:A:753:ASN:HB2	1:A:771:GLY:HA2	1.94	0.48
1:D:383:ASN:HA	5:D:8003:DMS:H12	1.96	0.48
1:A:246:MET:HG2	1:A:274:PHE:CE1	2.49	0.48
1:C:540:HIS:NE2	2:C:2001:149:H61	2.29	0.47
1:A:881:ARG:HE	1:A:987:ASP:CG	2.23	0.47
1:D:142:ILE:HG23	1:D:170:GLU:HG2	1.97	0.47
1:B:88:SER:HA	1:B:366:VAL:HG21	1.97	0.47
1:C:623:GLN:NE2	5:C:8002:DMS:H12	2.30	0.47
1:C:881:ARG:HE	1:C:987:ASP:CG	2.23	0.46
1:D:626:PHE:HE1	5:D:8003:DMS:H12	1.81	0.46
1:C:390:SER:HA	1:C:391:HIS:HA	1.73	0.46
1:B:147:ASN:HA	1:B:148:SER:HA	1.62	0.46
1:C:147:ASN:HA	1:C:148:SER:HA	1.67	0.46
1:A:473:ARG:NH1	6:A:4337:HOH:O	2.45	0.46
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.80	0.46
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.50	0.46
1:C:521:LYS:NZ	6:C:4394:HOH:O	2.45	0.46
1:C:887:GLN:NE2	1:C:980:GLU:O	2.47	0.46
1:C:939:CYS:HA	1:C:956:GLN:HB3	1.98	0.46
1:C:34:ALA:HB2	5:C:8004:DMS:H12	1.99	0.45
5:B:8011:DMS:H23	1:C:478:VAL:HG22	1.98	0.45
1:D:461:GLU:OE1	2:D:2001:149:H2	2.17	0.45
1:A:789:LEU:CD1	1:A:993:ILE:HG22	2.47	0.45
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.52	0.45
1:A:749:ILE:HD11	1:A:836:ILE:HD11	1.99	0.45
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.16	0.45
1:C:351:ILE:HD13	1:C:534:ILE:HD13	1.98	0.45
1:A:527:PRO:HB3	1:B:339:ASN:O	2.17	0.45
1:A:907:PRO:HG2	1:A:990:HIS:O	2.17	0.45
1:B:789:LEU:O	1:B:793:ILE:HG12	2.16	0.45
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.46	0.45
1:A:487:GLU:HB3	6:A:4029:HOH:O	2.17	0.44
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.39	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HB2	5:A:8004:DMS:H12	1.99	0.44
1:A:292:ARG:NH1	6:A:4377:HOH:O	2.43	0.44
1:A:658:LEU:O	1:A:659:ASP:C	2.61	0.44
1:A:751:LEU:HD21	1:A:860:GLY:O	2.17	0.44
1:C:340:GLY:O	1:C:561:ARG:HG2	2.18	0.44
1:D:337:ILE:HA	1:D:341:LEU:O	2.17	0.44
1:A:88:SER:HA	1:A:366:VAL:HG21	1.98	0.44
1:D:568:TRP:CZ2	2:D:2001:149:H4	2.53	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.52	0.44
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.99	0.44
1:B:354:VAL:HG12	1:B:379:MET:HE3	2.00	0.44
1:C:331:GLY:O	5:C:8001:DMS:C1	2.66	0.44
1:C:381:GLN:O	1:C:621:LYS:HE3	2.17	0.44
1:D:656:VAL:HG21	1:D:685:LEU:HD22	2.00	0.44
1:A:319:ASP:OD1	6:A:4459:HOH:O	2.21	0.43
1:C:34:ALA:HB2	5:C:8004:DMS:C1	2.48	0.43
1:B:610:ASP:O	1:B:611:ARG:HB2	2.18	0.43
1:A:890:GLN:HE21	1:A:892:ALA:HB2	1.84	0.43
1:C:43:ARG:HD2	1:C:261:TRP:CE3	2.54	0.43
1:A:595:THR:HA	1:A:596:PRO:C	2.44	0.43
1:B:390:SER:HA	1:B:391:HIS:HA	1.75	0.43
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.43
1:C:1022:GLN:HB2	6:C:4455:HOH:O	2.18	0.43
1:D:610:ASP:O	1:D:611:ARG:HB2	2.17	0.43
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.88	0.43
1:B:881:ARG:HE	1:B:987:ASP:CG	2.27	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.43
1:C:90:TRP:CD1	1:C:90:TRP:C	2.96	0.42
1:A:390:SER:HA	1:A:391:HIS:HA	1.82	0.42
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.84	0.42
1:C:942:ARG:HA	1:C:953:GLY:O	2.20	0.42
1:D:142:ILE:HG12	1:D:170:GLU:HG2	2.02	0.42
1:B:786:ARG:NH2	1:B:991:MET:HE2	2.34	0.42
1:B:542:MET:HA	1:B:604:ASN:HA	2.01	0.42
1:C:786:ARG:NH2	1:C:991:MET:HE2	2.35	0.42
1:D:854:LYS:HA	1:D:867:THR:O	2.20	0.42
1:B:626:PHE:CE1	5:B:8003:DMS:H12	2.54	0.42
1:A:286:ALA:HB2	5:A:1024:DMS:H22	2.01	0.42
1:B:478:VAL:HG13	5:B:1024:DMS:H13	2.01	0.42
1:B:383:ASN:HA	5:B:8003:DMS:C1	2.50	0.42
1:B:548:GLY:HA2	6:B:4057:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ASN:HB3	1:C:945:ASN:HB2	2.02	0.42
1:A:240:LEU:C	1:A:240:LEU:HD23	2.45	0.42
1:C:333:ARG:NH1	5:C:8001:DMS:H11	2.35	0.42
1:D:147:ASN:HB3	1:D:206:SER:HA	2.02	0.42
1:A:333:ARG:HA	1:A:345:ASN:OD1	2.19	0.41
1:B:277:GLU:HG2	6:B:4431:HOH:O	2.20	0.41
1:D:88:SER:HA	1:D:366:VAL:HG21	2.02	0.41
5:B:8003:DMS:H13	6:B:4064:HOH:O	2.20	0.41
1:A:299:LYS:NZ	6:A:4479:HOH:O	2.36	0.41
1:B:487:GLU:HB3	6:B:4042:HOH:O	2.20	0.41
1:D:301:TRP:CH2	1:D:452:SER:HA	2.55	0.41
1:A:788:PRO:HD2	1:A:968:MET:HB2	2.02	0.41
1:C:863:GLN:HG2	1:C:1021:CYS:HB3	2.03	0.41
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.03	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.84	0.41
1:D:626:PHE:CE1	5:D:8003:DMS:H12	2.56	0.41
1:C:451:PRO:HA	5:C:8001:DMS:H23	2.02	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD3	1.94	0.41
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.21	0.41
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.56	0.41
1:B:367:MET:HA	1:B:367:MET:HE2	2.02	0.41
1:B:942:ARG:HA	1:B:953:GLY:O	2.21	0.41
1:C:111:PRO:HA	1:C:112:PRO:HA	1.83	0.41
1:D:147:ASN:HA	1:D:148:SER:HA	1.68	0.41
1:A:782:ASP:HB2	1:A:842:TRP:CZ2	2.56	0.40
1:C:147:ASN:HB3	1:C:206:SER:HA	2.03	0.40
1:A:353:GLY:HA2	1:A:386:ALA:O	2.21	0.40
1:C:907:PRO:HG2	1:C:990:HIS:O	2.22	0.40
1:D:225:PHE:HA	1:D:243:GLU:O	2.21	0.40
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	2.03	0.40
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.02	0.40
1:A:878:HIS:HD2	6:A:4048:HOH:O	2.04	0.40
1:A:896:ASN:HB3	1:A:945:ASN:HB2	2.04	0.40
1:D:139:THR:OG1	1:D:216:HIS:HD2	2.03	0.40
1:D:786:ARG:NH2	1:D:991:MET:HE2	2.36	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%)	973 (96%)	40 (4%)	0	100	100
1	B	1013/1052 (96%)	971 (96%)	41 (4%)	1 (0%)	48	64
1	C	1013/1052 (96%)	972 (96%)	41 (4%)	0	100	100
1	D	1013/1052 (96%)	966 (95%)	47 (5%)	0	100	100
All	All	4052/4208 (96%)	3882 (96%)	169 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	794	GLY

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%)	853 (98%)	15 (2%)	53	74
1	B	868/898 (97%)	857 (99%)	11 (1%)	61	80
1	C	868/898 (97%)	856 (99%)	12 (1%)	59	79
1	D	868/898 (97%)	851 (98%)	17 (2%)	48	70
All	All	3472/3592 (97%)	3417 (98%)	55 (2%)	55	76

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	80	GLU
1	A	189	LEU
1	A	245	GLN
1	A	319	ASP
1	A	519	SER
1	A	546	LEU
1	A	652	LEU
1	A	663	LEU
1	A	672	VAL
1	A	685	LEU
1	A	737	ILE
1	A	745	MET
1	A	772	ASP
1	A	956	GLN
1	B	76	CYS
1	B	80	GLU
1	B	135	GLN
1	B	344	LEU
1	B	351	ILE
1	B	546	LEU
1	B	672	VAL
1	B	689	GLU
1	B	795	VAL
1	B	956	GLN
1	B	1022	GLN
1	C	80	GLU
1	C	264	GLU
1	C	344	LEU
1	C	351	ILE
1	C	478	VAL
1	C	519	SER
1	C	546	LEU
1	C	672	VAL
1	C	680	ILE
1	C	766	SER
1	C	956	GLN
1	C	1022	GLN
1	D	75	GLU
1	D	80	GLU
1	D	299	LYS
1	D	344	LEU
1	D	351	ILE

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Mol	Chain	Res	Type
1	D	371	THR
1	D	478	VAL
1	D	519	SER
1	D	546	LEU
1	D	663	LEU
1	D	672	VAL
1	D	685	LEU
1	D	743	SER
1	D	755	ARG
1	D	796	ASP
1	D	850	PHE
1	D	956	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	128	ASN
1	A	262	GLN
1	A	445	GLN
1	A	485	GLN
1	A	554	GLN
1	A	558	GLN
1	A	634	GLN
1	A	693	GLN
1	A	817	GLN
1	A	878	HIS
1	A	1022	GLN
1	B	50	GLN
1	B	266	GLN
1	B	294	ASN
1	B	485	GLN
1	B	634	GLN
1	B	693	GLN
1	B	702	GLN
1	B	718	GLN
1	B	824	GLN
1	B	878	HIS
1	B	1022	GLN
1	C	445	GLN
1	C	485	GLN
1	C	597	ASN

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Mol	Chain	Res	Type
1	C	623	GLN
1	C	693	GLN
1	C	702	GLN
1	C	817	GLN
1	C	878	HIS
1	C	885	ASN
1	C	974	HIS
1	D	216	HIS
1	D	262	GLN
1	D	297	ASN
1	D	363	HIS
1	D	394	ASN
1	D	445	GLN
1	D	581	ASN
1	D	702	GLN
1	D	757	GLN
1	D	783	GLN
1	D	824	GLN
1	D	843	GLN
1	D	885	ASN
1	D	985	ASN
1	D	1017	GLN
1	D	1022	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 19 are monoatomic - leaving 53 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	A	8009	-	3,3,3	2.75	1 (33%)	3,3,3	0.66	0
5	DMS	A	8001	-	3,3,3	2.62	1 (33%)	3,3,3	1.01	0
5	DMS	A	8002	-	3,3,3	2.52	1 (33%)	3,3,3	0.53	0
5	DMS	D	8001	-	3,3,3	2.64	1 (33%)	3,3,3	0.86	0
5	DMS	C	8008	-	3,3,3	2.74	1 (33%)	3,3,3	0.71	0
5	DMS	B	8008	-	3,3,3	2.72	1 (33%)	3,3,3	0.84	0
5	DMS	B	8009	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
5	DMS	C	8001	-	3,3,3	2.65	1 (33%)	3,3,3	0.89	0
5	DMS	A	8003	-	3,3,3	2.68	1 (33%)	3,3,3	0.76	0
5	DMS	B	8006	-	3,3,3	2.71	1 (33%)	3,3,3	0.58	0
5	DMS	A	8004	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
5	DMS	D	8003	-	3,3,3	2.73	1 (33%)	3,3,3	0.73	0
5	DMS	D	8004	-	3,3,3	2.71	1 (33%)	3,3,3	0.57	0
5	DMS	D	8007	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
5	DMS	C	8002	-	3,3,3	2.64	1 (33%)	3,3,3	0.68	0
5	DMS	A	1024	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
5	DMS	B	8001	-	3,3,3	2.58	1 (33%)	3,3,3	0.71	0
2	149	A	2001	4	12,12,12	2.44	2 (16%)	15,17,17	0.88	0
2	149	D	2001	4	12,12,12	2.39	2 (16%)	15,17,17	0.73	0
5	DMS	A	8012	-	3,3,3	2.78	1 (33%)	3,3,3	0.66	0
5	DMS	A	8008	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
5	DMS	C	8013	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
5	DMS	A	8005	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
5	DMS	D	8006	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
5	DMS	B	8010	-	3,3,3	2.70	1 (33%)	3,3,3	0.71	0
2	149	B	2001	4	12,12,12	2.64	1 (8%)	15,17,17	0.97	1 (6%)
5	DMS	B	8012	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
5	DMS	D	8009	-	3,3,3	2.76	1 (33%)	3,3,3	0.68	0
5	DMS	C	8011	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8011	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
5	DMS	D	8008	-	3,3,3	2.66	1 (33%)	3,3,3	0.63	0
5	DMS	A	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.80	0
5	DMS	C	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
5	DMS	C	8012	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
2	149	C	2001	4	12,12,12	2.48	2 (16%)	15,17,17	0.79	1 (6%)
5	DMS	D	8005	-	3,3,3	2.55	1 (33%)	3,3,3	0.65	0
5	DMS	B	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
5	DMS	A	8010	-	3,3,3	2.72	1 (33%)	3,3,3	0.88	0
5	DMS	A	8007	-	3,3,3	2.75	1 (33%)	3,3,3	0.51	0
5	DMS	B	8013	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
5	DMS	C	8009	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
5	DMS	D	8002	-	3,3,3	2.59	1 (33%)	3,3,3	0.62	0
5	DMS	B	8002	-	3,3,3	2.59	1 (33%)	3,3,3	0.81	0
5	DMS	B	8004	-	3,3,3	2.70	1 (33%)	3,3,3	0.63	0
5	DMS	A	8011	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
5	DMS	C	8005	-	3,3,3	2.67	1 (33%)	3,3,3	0.29	0
5	DMS	C	8006	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
5	DMS	B	1024	-	3,3,3	2.67	1 (33%)	3,3,3	0.37	0
5	DMS	B	8003	-	3,3,3	2.73	1 (33%)	3,3,3	0.64	0
5	DMS	C	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
5	DMS	C	8004	-	3,3,3	2.78	1 (33%)	3,3,3	0.73	0
5	DMS	B	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.38	0
5	DMS	B	8014	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	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	-	2/2/22/22	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
2	149	C	2001	4	-	1/2/22/22	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	149	O5-C1	8.85	1.47	1.34
2	C	2001	149	O5-C1	8.10	1.46	1.34
2	A	2001	149	O5-C1	8.07	1.46	1.34
2	D	2001	149	O5-C1	7.88	1.46	1.34
5	C	8004	DMS	O-S	4.67	1.81	1.50
5	A	8012	DMS	O-S	4.66	1.81	1.50
5	C	8006	DMS	O-S	4.62	1.80	1.50
5	D	8006	DMS	O-S	4.62	1.80	1.50
5	D	8009	DMS	O-S	4.62	1.80	1.50
5	A	8009	DMS	O-S	4.61	1.80	1.50
5	C	8011	DMS	O-S	4.61	1.80	1.50
5	A	8007	DMS	O-S	4.61	1.80	1.50
5	B	8003	DMS	O-S	4.60	1.80	1.50
5	C	8008	DMS	O-S	4.59	1.80	1.50
5	A	8004	DMS	O-S	4.59	1.80	1.50
5	A	8006	DMS	O-S	4.59	1.80	1.50
5	A	1024	DMS	O-S	4.59	1.80	1.50
5	D	8003	DMS	O-S	4.58	1.80	1.50
5	C	8007	DMS	O-S	4.58	1.80	1.50
5	B	8008	DMS	O-S	4.56	1.80	1.50
5	D	8007	DMS	O-S	4.56	1.80	1.50
5	A	8008	DMS	O-S	4.56	1.80	1.50
5	B	8014	DMS	O-S	4.56	1.80	1.50
5	A	8011	DMS	O-S	4.55	1.80	1.50
5	B	8013	DMS	O-S	4.55	1.80	1.50
5	D	8004	DMS	O-S	4.54	1.80	1.50
5	B	8006	DMS	O-S	4.54	1.80	1.50
5	C	8012	DMS	O-S	4.54	1.80	1.50
5	A	8010	DMS	O-S	4.54	1.80	1.50
5	B	8004	DMS	O-S	4.53	1.80	1.50
5	C	8003	DMS	O-S	4.53	1.80	1.50
5	C	8009	DMS	O-S	4.53	1.80	1.50
5	B	8009	DMS	O-S	4.52	1.80	1.50
5	C	8013	DMS	O-S	4.51	1.80	1.50
5	A	8003	DMS	O-S	4.50	1.79	1.50
5	B	8010	DMS	O-S	4.50	1.79	1.50
5	B	8012	DMS	O-S	4.50	1.79	1.50
5	B	1024	DMS	O-S	4.48	1.79	1.50
5	B	8011	DMS	O-S	4.47	1.79	1.50
5	B	8007	DMS	O-S	4.47	1.79	1.50
5	A	8005	DMS	O-S	4.47	1.79	1.50
5	C	8005	DMS	O-S	4.47	1.79	1.50
5	C	8001	DMS	O-S	4.47	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8002	DMS	O-S	4.45	1.79	1.50
5	D	8008	DMS	O-S	4.43	1.79	1.50
5	B	8005	DMS	O-S	4.42	1.79	1.50
5	D	8001	DMS	O-S	4.40	1.79	1.50
5	A	8001	DMS	O-S	4.40	1.79	1.50
5	D	8002	DMS	O-S	4.34	1.78	1.50
5	B	8002	DMS	O-S	4.33	1.78	1.50
5	B	8001	DMS	O-S	4.33	1.78	1.50
5	D	8005	DMS	O-S	4.25	1.78	1.50
5	A	8002	DMS	O-S	4.22	1.78	1.50
2	C	2001	149	O5-C5	-2.33	1.43	1.46
2	D	2001	149	O5-C5	-2.20	1.43	1.46
2	A	2001	149	O5-C5	-2.16	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	149	O5-C1-C2	2.83	123.41	119.14
2	C	2001	149	O5-C1-C2	2.04	122.21	119.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	149	O5-C5-C6-O6
2	A	2001	149	O5-C5-C6-O6
2	B	2001	149	C4-C5-C6-O6
2	D	2001	149	O5-C5-C6-O6
2	C	2001	149	O5-C5-C6-O6

There are no ring outliers.

22 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8009	DMS	1	0
5	D	8001	DMS	1	0
5	C	8008	DMS	1	0
5	B	8008	DMS	1	0
5	C	8001	DMS	4	0
5	A	8003	DMS	2	0
5	A	8004	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8003	DMS	4	0
5	C	8002	DMS	1	0
5	A	1024	DMS	1	0
5	B	8001	DMS	1	0
2	D	2001	149	2	0
5	A	8005	DMS	3	0
5	B	8011	DMS	1	0
5	C	8003	DMS	3	0
2	C	2001	149	3	0
5	A	8010	DMS	1	0
5	B	8013	DMS	1	0
5	C	8009	DMS	1	0
5	B	1024	DMS	1	0
5	B	8003	DMS	6	0
5	C	8004	DMS	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1008/1052 (95%)	-0.04	34 (3%)	48	44	23, 44, 80, 113	0
1	B	1006/1052 (95%)	-0.11	22 (2%)	62	58	23, 43, 73, 113	0
1	C	1006/1052 (95%)	0.03	37 (3%)	45	41	24, 44, 77, 123	0
1	D	1006/1052 (95%)	0.12	41 (4%)	41	37	25, 47, 82, 121	0
All	All	4026/4208 (95%)	-0.00	134 (3%)	49	45	23, 44, 79, 123	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	5.3
1	D	9	VAL	5.2
1	A	11	LEU	4.8
1	A	9	VAL	4.6
1	D	686	PRO	4.6
1	C	596	PRO	4.4
1	D	10	VAL	4.2
1	D	596	PRO	4.2
1	A	10	VAL	4.2
1	C	582	GLY	4.1
1	A	931	PHE	4.0
1	C	686	PRO	3.9
1	A	772	ASP	3.8
1	A	596	PRO	3.8
1	B	10	VAL	3.7
1	C	595	THR	3.7
1	D	803	PRO	3.7
1	C	731	PRO	3.7
1	C	730	LEU	3.5
1	B	1023	LYS	3.5
1	B	686	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	3.4
1	B	731	PRO	3.4
1	D	733	ALA	3.4
1	A	730	LEU	3.4
1	C	736	ALA	3.4
1	C	583	ASN	3.4
1	B	11	LEU	3.3
1	C	10	VAL	3.3
1	D	685	LEU	3.2
1	B	730	LEU	3.1
1	A	794	GLY	3.1
1	A	76	CYS	3.0
1	B	803	PRO	3.0
1	D	737	ILE	3.0
1	B	685	LEU	3.0
1	C	733	ALA	2.9
1	D	594	ASP	2.9
1	B	9	VAL	2.9
1	B	753	ASN	2.9
1	C	737	ILE	2.9
1	D	770	ILE	2.9
1	A	77	ASP	2.9
1	B	770	ILE	2.8
1	A	600	GLN	2.8
1	A	588	TYR	2.8
1	B	745	MET	2.8
1	C	579	ASP	2.7
1	D	931	PHE	2.7
1	D	734	SER	2.7
1	D	730	LEU	2.7
1	C	745	MET	2.7
1	C	685	LEU	2.7
1	D	11	LEU	2.7
1	D	732	ALA	2.7
1	D	741	THR	2.7
1	B	76	CYS	2.6
1	A	773	LYS	2.6
1	B	688	PRO	2.6
1	C	831	ALA	2.6
1	C	770	ILE	2.6
1	A	732	ALA	2.6
1	D	592	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	685	LEU	2.5
1	C	1022	GLN	2.5
1	C	688	PRO	2.5
1	B	596	PRO	2.5
1	D	688	PRO	2.5
1	B	1022	GLN	2.4
1	C	734	SER	2.4
1	A	603	MET	2.4
1	C	1023	LYS	2.4
1	B	752	GLY	2.4
1	D	600	GLN	2.4
1	C	9	VAL	2.4
1	A	65	ALA	2.4
1	A	604	ASN	2.4
1	A	735	HIS	2.3
1	D	74	LEU	2.3
1	D	130	ASP	2.3
1	D	76	CYS	2.3
1	C	588	TYR	2.3
1	A	594	ASP	2.3
1	D	735	HIS	2.3
1	C	793	ILE	2.3
1	A	598	ASP	2.3
1	C	580	GLU	2.3
1	A	688	PRO	2.3
1	C	732	ALA	2.3
1	B	595	THR	2.3
1	D	1023	LYS	2.2
1	C	594	ASP	2.2
1	B	755	ARG	2.2
1	C	584	PRO	2.2
1	D	736	ALA	2.2
1	A	1023	LYS	2.2
1	D	604	ASN	2.2
1	C	739	HIS	2.2
1	D	653	HIS	2.2
1	A	595	THR	2.2
1	A	998	SER	2.2
1	D	77	ASP	2.2
1	D	774	LYS	2.2
1	D	588	TYR	2.2
1	D	593	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	79	PRO	2.2
1	C	977	HIS	2.1
1	A	126	THR	2.1
1	D	663	LEU	2.1
1	D	578	TYR	2.1
1	D	731	PRO	2.1
1	D	85	VAL	2.1
1	D	793	ILE	2.1
1	A	71	GLU	2.1
1	A	578	TYR	2.1
1	A	774	LYS	2.1
1	A	584	PRO	2.1
1	C	735	HIS	2.1
1	B	732	ALA	2.1
1	B	769	TRP	2.1
1	C	740	LEU	2.1
1	C	998	SER	2.1
1	A	731	PRO	2.1
1	D	79	PRO	2.1
1	D	64	PRO	2.1
1	A	68	ALA	2.0
1	B	663	LEU	2.0
1	C	78	LEU	2.0
1	D	71	GLU	2.0
1	C	999	TRP	2.0
1	D	595	THR	2.0
1	C	598	ASP	2.0
1	C	604	ASN	2.0
1	D	977	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	D	3101	1/1	0.65	0.18	83,83,83,83	0
4	NA	A	3101	1/1	0.70	0.22	83,83,83,83	0
4	NA	B	3101	1/1	0.77	0.16	64,64,64,64	0
5	DMS	A	1024	4/4	0.77	0.28	87,88,89,91	0
5	DMS	B	1024	4/4	0.81	0.24	75,76,76,76	0
5	DMS	B	8009	4/4	0.82	0.27	101,101,103,103	0
4	NA	C	3101	1/1	0.83	0.13	63,63,63,63	0
5	DMS	C	8004	4/4	0.84	0.26	72,75,76,78	0
5	DMS	C	8006	4/4	0.84	0.22	110,110,111,112	0
5	DMS	C	8011	4/4	0.86	0.23	99,100,101,103	0
5	DMS	A	8011	4/4	0.87	0.24	88,91,91,91	0
5	DMS	B	8005	4/4	0.87	0.21	62,66,66,66	0
5	DMS	C	8007	4/4	0.87	0.22	82,82,83,84	0
5	DMS	B	8012	4/4	0.87	0.21	79,79,79,83	0
2	149	A	2001	12/12	0.88	0.15	71,84,87,91	0
5	DMS	B	8006	4/4	0.88	0.24	97,97,98,98	0
5	DMS	A	8010	4/4	0.88	0.21	78,78,80,82	0
5	DMS	B	8008	4/4	0.89	0.19	66,69,70,76	0
5	DMS	A	8012	4/4	0.89	0.17	68,68,72,72	0
5	DMS	A	8009	4/4	0.89	0.17	68,72,73,74	0
2	149	D	2001	12/12	0.89	0.15	65,80,89,91	0
5	DMS	C	8012	4/4	0.89	0.18	73,73,74,75	0
5	DMS	D	8004	4/4	0.89	0.22	68,70,73,77	0
5	DMS	D	8006	4/4	0.89	0.21	71,73,76,76	0
5	DMS	D	8009	4/4	0.89	0.17	56,65,68,69	0
5	DMS	C	8008	4/4	0.90	0.18	69,70,71,79	0
5	DMS	B	8011	4/4	0.90	0.23	81,81,82,84	0
2	149	C	2001	12/12	0.90	0.13	57,67,76,77	0
2	149	B	2001	12/12	0.90	0.12	43,63,66,73	0
5	DMS	B	8004	4/4	0.90	0.20	57,63,64,65	0
5	DMS	A	8004	4/4	0.90	0.19	71,75,77,78	0
5	DMS	C	8013	4/4	0.91	0.19	89,90,90,91	0
5	DMS	B	8010	4/4	0.91	0.18	65,68,69,70	0
4	NA	C	3104	1/1	0.91	0.09	58,58,58,58	0
5	DMS	B	8013	4/4	0.91	0.17	57,60,60,61	0
5	DMS	A	8007	4/4	0.92	0.16	58,58,60,61	0
4	NA	A	3103	1/1	0.92	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	8002	4/4	0.92	0.17	56,62,62,65	0
3	MG	C	3002	1/1	0.92	0.10	43,43,43,43	0
5	DMS	D	8005	4/4	0.92	0.18	56,62,63,64	0
5	DMS	A	8006	4/4	0.92	0.18	68,69,70,72	0
5	DMS	D	8007	4/4	0.92	0.15	66,67,67,71	0
5	DMS	B	8014	4/4	0.92	0.15	63,65,68,68	0
5	DMS	B	8002	4/4	0.94	0.16	43,51,56,57	0
4	NA	B	3104	1/1	0.94	0.08	53,53,53,53	0
5	DMS	D	8008	4/4	0.94	0.14	55,57,62,65	0
5	DMS	B	8007	4/4	0.94	0.14	61,64,67,69	0
5	DMS	A	8002	4/4	0.95	0.13	48,50,52,56	0
5	DMS	A	8003	4/4	0.95	0.15	52,54,57,59	0
5	DMS	D	8001	4/4	0.95	0.12	45,50,53,56	0
3	MG	A	3002	1/1	0.95	0.09	44,44,44,44	0
5	DMS	C	8005	4/4	0.95	0.12	50,51,52,55	0
3	MG	D	3002	1/1	0.96	0.10	51,51,51,51	0
5	DMS	A	8008	4/4	0.96	0.12	59,62,62,62	0
5	DMS	B	8003	4/4	0.96	0.13	55,60,60,66	0
5	DMS	C	8001	4/4	0.96	0.12	42,48,50,53	0
5	DMS	C	8009	4/4	0.96	0.11	56,61,64,66	0
5	DMS	C	8002	4/4	0.96	0.13	54,59,60,61	0
5	DMS	C	8003	4/4	0.96	0.12	55,59,59,61	0
3	MG	B	3002	1/1	0.96	0.11	38,38,38,38	0
3	MG	C	3001	1/1	0.97	0.05	44,44,44,44	0
4	NA	C	3102	1/1	0.97	0.05	32,32,32,32	0
4	NA	D	3102	1/1	0.97	0.06	35,35,35,35	0
5	DMS	A	8005	4/4	0.97	0.11	55,58,61,63	0
5	DMS	A	8001	4/4	0.97	0.11	43,45,47,53	0
5	DMS	D	8003	4/4	0.97	0.13	51,54,54,54	0
5	DMS	B	8001	4/4	0.98	0.09	38,45,47,51	0
3	MG	D	3001	1/1	0.98	0.06	43,43,43,43	0
4	NA	B	3102	1/1	0.98	0.04	34,34,34,34	0
3	MG	A	3001	1/1	0.98	0.06	43,43,43,43	0
3	MG	B	3001	1/1	0.99	0.03	41,41,41,41	0
4	NA	A	3102	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.