



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:55 AM UTC

PDB ID : 3SEP / pdb_00003sep
Title : E. coli (lacZ) beta-galactosidase (S796A)
Authors : Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.
Deposited on : 2011-06-10
Resolution : 2.05 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

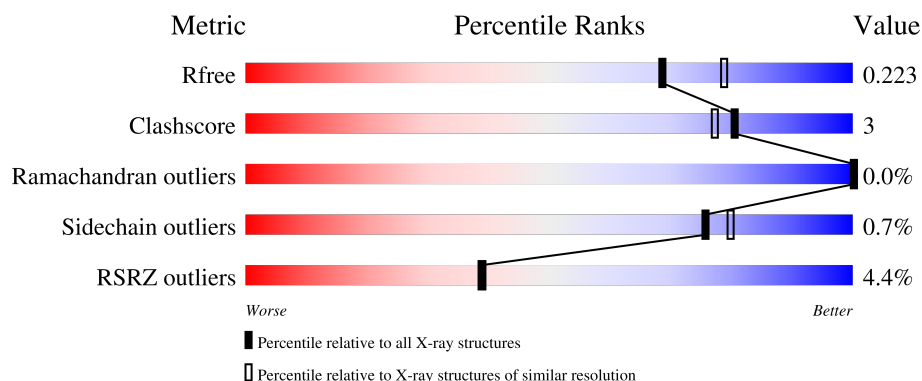
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

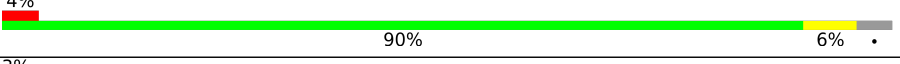
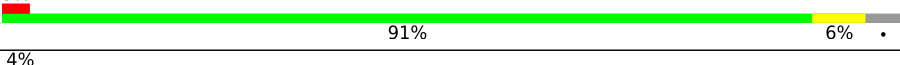
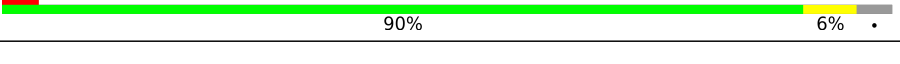
The reported resolution of this entry is 2.05 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-galactosidase.

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

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P00722
A	-27	GLY	-	expression tag	UNP P00722
A	-26	GLY	-	expression tag	UNP P00722
A	-25	SER	-	expression tag	UNP P00722
A	-24	HIS	-	expression tag	UNP P00722
A	-23	HIS	-	expression tag	UNP P00722
A	-22	HIS	-	expression tag	UNP P00722
A	-21	HIS	-	expression tag	UNP P00722
A	-20	HIS	-	expression tag	UNP P00722
A	-19	HIS	-	expression tag	UNP P00722
A	-18	GLY	-	expression tag	UNP P00722
A	-17	MET	-	expression tag	UNP P00722
A	-16	ALA	-	expression tag	UNP P00722
A	-15	SER	-	expression tag	UNP P00722
A	-14	MET	-	expression tag	UNP P00722
A	-13	THR	-	expression tag	UNP P00722
A	-12	GLY	-	expression tag	UNP P00722
A	-11	GLY	-	expression tag	UNP P00722
A	-10	GLN	-	expression tag	UNP P00722
A	-9	GLN	-	expression tag	UNP P00722
A	-8	MET	-	expression tag	UNP P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P00722
A	-6	ARG	-	expression tag	UNP P00722
A	-5	ASP	-	expression tag	UNP P00722
A	-4	LEU	-	expression tag	UNP P00722
A	-3	TYR	-	expression tag	UNP P00722
A	-2	ASP	-	expression tag	UNP P00722
A	-1	ASP	-	expression tag	UNP P00722
A	0	ASP	-	expression tag	UNP P00722
A	1	ASP	-	expression tag	UNP P00722
A	2	LYS	-	expression tag	UNP P00722
A	3	ASP	-	expression tag	UNP P00722
A	4	PRO	-	expression tag	UNP P00722
A	5	MET	-	expression tag	UNP P00722
A	6	ILE	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	796	ALA	SER	engineered mutation	UNP P00722
B	-28	MET	-	expression tag	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	TYR	-	expression tag	UNP P00722
B	-2	ASP	-	expression tag	UNP P00722
B	-1	ASP	-	expression tag	UNP P00722
B	0	ASP	-	expression tag	UNP P00722
B	1	ASP	-	expression tag	UNP P00722
B	2	LYS	-	expression tag	UNP P00722
B	3	ASP	-	expression tag	UNP P00722
B	4	PRO	-	expression tag	UNP P00722
B	5	MET	-	expression tag	UNP P00722
B	6	ILE	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	796	ALA	SER	engineered mutation	UNP P00722
C	-28	MET	-	expression tag	UNP P00722
C	-27	GLY	-	expression tag	UNP P00722
C	-26	GLY	-	expression tag	UNP P00722
C	-25	SER	-	expression tag	UNP P00722
C	-24	HIS	-	expression tag	UNP P00722
C	-23	HIS	-	expression tag	UNP P00722
C	-22	HIS	-	expression tag	UNP P00722
C	-21	HIS	-	expression tag	UNP P00722
C	-20	HIS	-	expression tag	UNP P00722
C	-19	HIS	-	expression tag	UNP P00722
C	-18	GLY	-	expression tag	UNP P00722
C	-17	MET	-	expression tag	UNP P00722
C	-16	ALA	-	expression tag	UNP P00722
C	-15	SER	-	expression tag	UNP P00722
C	-14	MET	-	expression tag	UNP P00722
C	-13	THR	-	expression tag	UNP P00722
C	-12	GLY	-	expression tag	UNP P00722
C	-11	GLY	-	expression tag	UNP P00722
C	-10	GLN	-	expression tag	UNP P00722
C	-9	GLN	-	expression tag	UNP P00722
C	-8	MET	-	expression tag	UNP P00722
C	-7	GLY	-	expression tag	UNP P00722
C	-6	ARG	-	expression tag	UNP P00722
C	-5	ASP	-	expression tag	UNP P00722
C	-4	LEU	-	expression tag	UNP P00722
C	-3	TYR	-	expression tag	UNP P00722
C	-2	ASP	-	expression tag	UNP P00722
C	-1	ASP	-	expression tag	UNP P00722
C	0	ASP	-	expression tag	UNP P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	796	ALA	SER	engineered mutation	UNP P00722
D	-28	MET	-	expression tag	UNP P00722
D	-27	GLY	-	expression tag	UNP P00722
D	-26	GLY	-	expression tag	UNP P00722
D	-25	SER	-	expression tag	UNP P00722
D	-24	HIS	-	expression tag	UNP P00722
D	-23	HIS	-	expression tag	UNP P00722
D	-22	HIS	-	expression tag	UNP P00722
D	-21	HIS	-	expression tag	UNP P00722
D	-20	HIS	-	expression tag	UNP P00722
D	-19	HIS	-	expression tag	UNP P00722
D	-18	GLY	-	expression tag	UNP P00722
D	-17	MET	-	expression tag	UNP P00722
D	-16	ALA	-	expression tag	UNP P00722
D	-15	SER	-	expression tag	UNP P00722
D	-14	MET	-	expression tag	UNP P00722
D	-13	THR	-	expression tag	UNP P00722
D	-12	GLY	-	expression tag	UNP P00722
D	-11	GLY	-	expression tag	UNP P00722
D	-10	GLN	-	expression tag	UNP P00722
D	-9	GLN	-	expression tag	UNP P00722
D	-8	MET	-	expression tag	UNP P00722
D	-7	GLY	-	expression tag	UNP P00722
D	-6	ARG	-	expression tag	UNP P00722
D	-5	ASP	-	expression tag	UNP P00722
D	-4	LEU	-	expression tag	UNP P00722
D	-3	TYR	-	expression tag	UNP P00722
D	-2	ASP	-	expression tag	UNP P00722
D	-1	ASP	-	expression tag	UNP P00722
D	0	ASP	-	expression tag	UNP P00722
D	1	ASP	-	expression tag	UNP P00722
D	2	LYS	-	expression tag	UNP P00722
D	3	ASP	-	expression tag	UNP P00722
D	4	PRO	-	expression tag	UNP P00722

Continued on next page...

Continued from previous page...

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

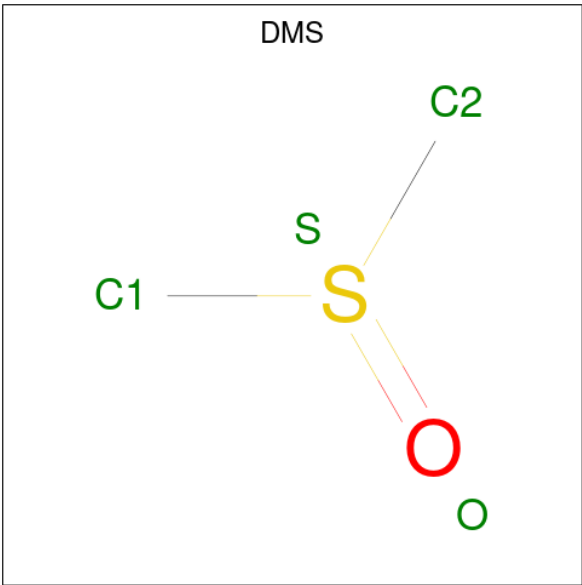
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

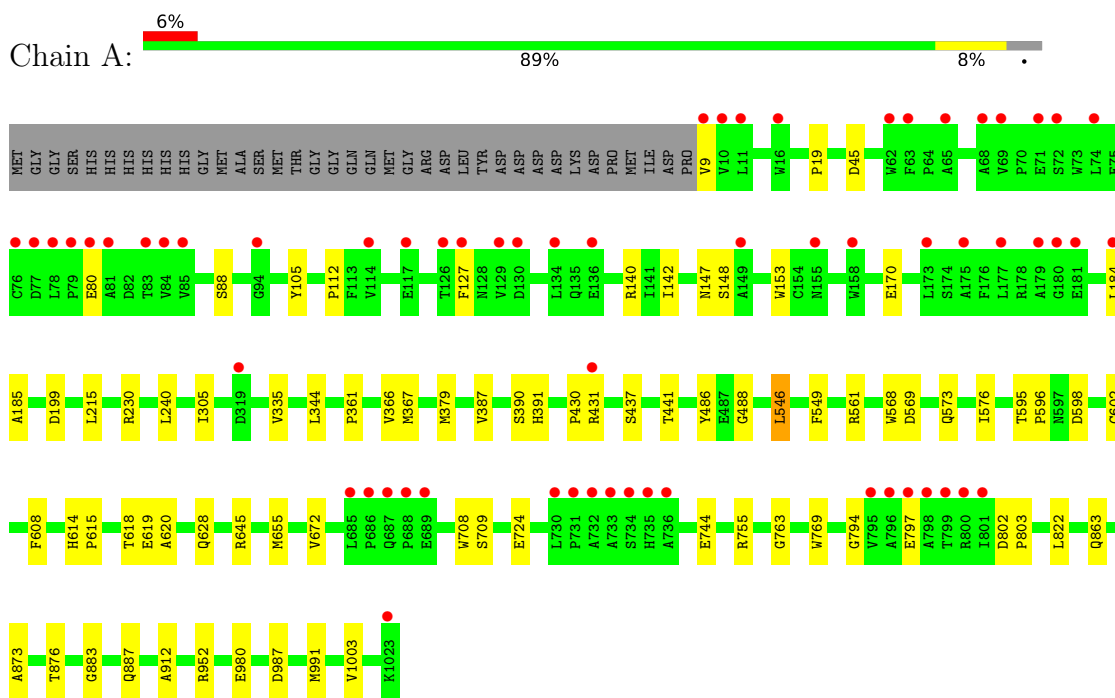
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	910	Total	O	0	0
			910	910		
5	B	1130	Total	O	0	0
			1130	1130		
5	C	1120	Total	O	0	0
			1120	1120		
5	D	925	Total	O	0	0
			925	925		

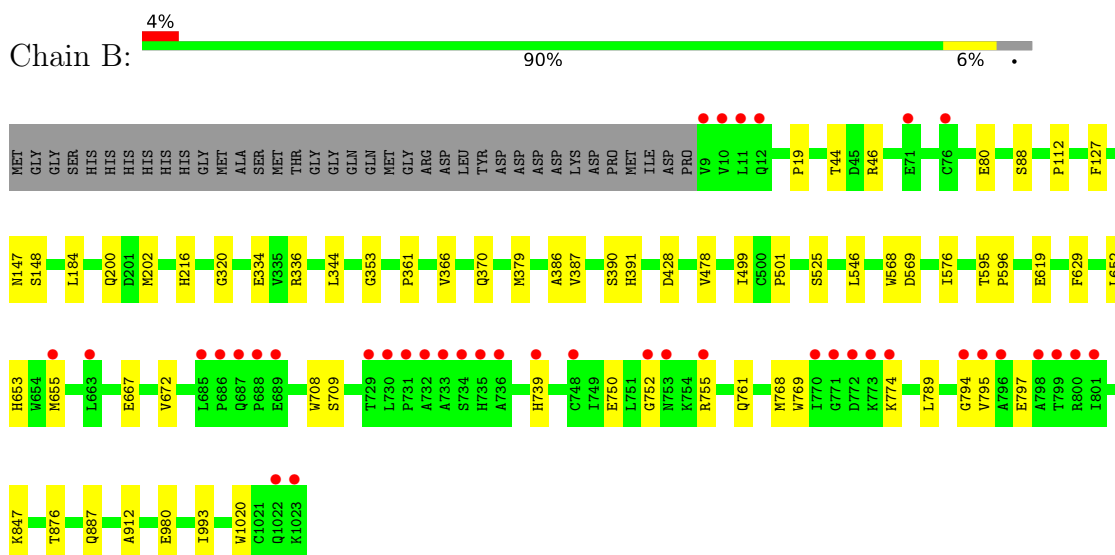
3 Residue-property plots

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.

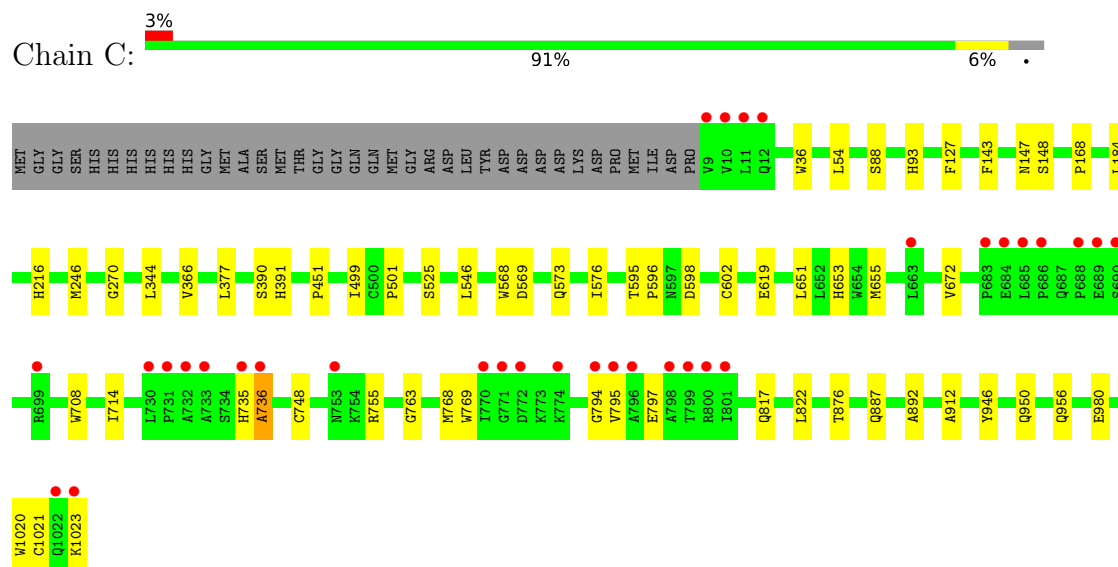
• Molecule 1: Beta-galactosidase



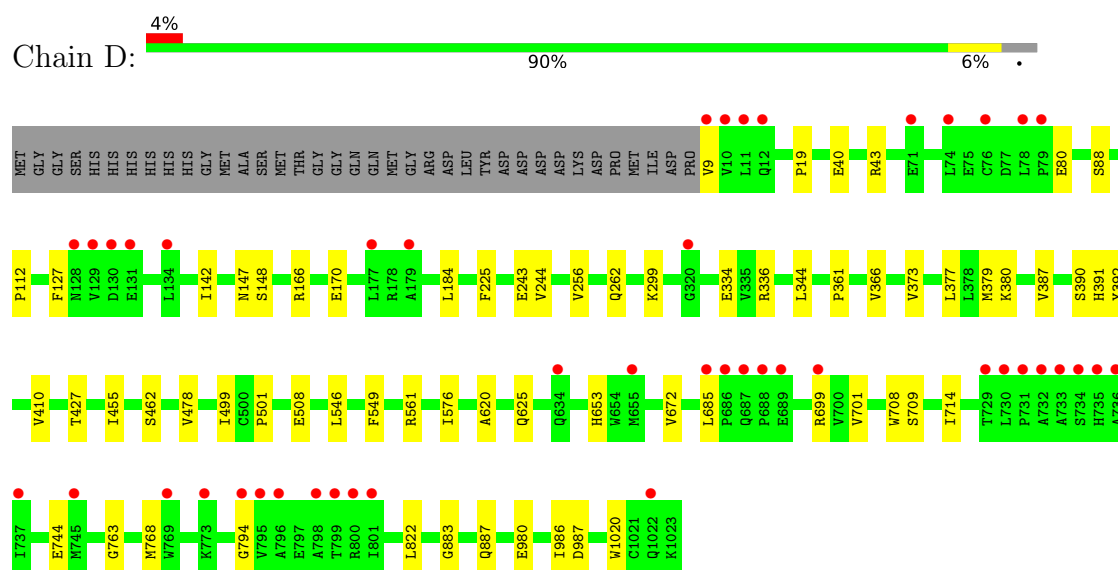
• Molecule 1: Beta-galactosidase



- 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	152.34Å 163.16Å 203.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.05 80.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.00-2.05) 90.1 (80.00-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.172 , 0.221 0.175 , 0.223	Depositor DCC
R_{free} test set	4086 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37044	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 39.98 % 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 2.9261e-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, 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	0.47	0/8398	0.71	0/11457
1	B	0.49	0/8398	0.70	0/11457
1	C	0.49	0/8398	0.70	0/11457
1	D	0.45	0/8398	0.70	0/11457
All	All	0.48	0/33592	0.70	0/45828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	8156	0	7753	47	0
1	B	8156	0	7753	36	0
1	C	8156	0	7753	38	0
1	D	8156	0	7753	43	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	84	0	126	5	0
4	B	92	0	138	4	0
4	C	80	0	120	11	0
4	D	56	0	84	9	0
5	A	910	0	0	6	0
5	B	1130	0	0	5	0
5	C	1120	0	0	5	0
5	D	925	0	0	4	0
All	All	37044	0	31480	166	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 (166) 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)
4:C:8003:DMS:H21	5:C:4238:HOH:O	1.75	0.86
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.60	0.84
1:C:887:GLN:NE2	1:C:980:GLU:O	2.13	0.81
1:D:699:ARG:HH12	4:D:8012:DMS:H12	1.52	0.74
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.25	0.71
1:C:735:HIS:O	1:C:736:ALA:HB3	1.97	0.64
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.33	0.64
4:D:8004:DMS:O	4:D:8013:DMS:H12	1.99	0.61
1:C:735:HIS:O	1:C:736:ALA:CB	2.48	0.61
1:D:887:GLN:NE2	1:D:980:GLU:O	2.32	0.61
1:C:655:MET:HB2	5:C:4796:HOH:O	2.00	0.61
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.65	0.60
1:D:262:GLN:HE22	1:D:299:LYS:CE	2.14	0.60
1:C:54:LEU:HA	4:C:8007:DMS:H12	1.84	0.60
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.84	0.59
4:D:8002:DMS:H22	5:D:4044:HOH:O	2.03	0.58
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.38	0.58
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.67	0.57
1:D:653:HIS:HD2	1:D:701:VAL:HG21	1.69	0.57
4:D:8003:DMS:H13	5:D:4103:HOH:O	2.04	0.57
1:A:655:MET:HB2	5:A:4752:HOH:O	2.04	0.56
1:C:216:HIS:ND1	4:C:8020:DMS:H13	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.41	0.56
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.88	0.55
1:D:262:GLN:HE22	1:D:299:LYS:HE2	1.71	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.54
1:B:887:GLN:NE2	1:B:980:GLU:O	2.36	0.54
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.43	0.54
1:D:262:GLN:NE2	1:D:299:LYS:CE	2.70	0.54
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.90	0.53
1:B:739:HIS:HB2	5:B:4995:HOH:O	2.09	0.53
1:C:950:GLN:HB2	1:C:1023:LYS:HB3	1.90	0.53
1:A:863:GLN:OE1	1:A:952:ARG:NH2	2.42	0.52
1:B:655:MET:HB2	5:B:4878:HOH:O	2.08	0.52
1:A:431:ARG:NH2	5:A:4394:HOH:O	2.41	0.52
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.45	0.52
1:C:270:GLY:HA3	4:C:8005:DMS:O	2.09	0.51
1:A:379:MET:HE1	1:A:387:VAL:HB	1.92	0.51
1:B:478:VAL:HG22	4:C:8014:DMS:H13	1.92	0.51
1:C:748:CYS:HB3	5:C:5091:HOH:O	2.11	0.51
1:A:608:PHE:CE2	1:A:614:HIS:HD2	2.29	0.51
1:C:598:ASP:OD1	1:C:797:GLU:HA	2.11	0.51
1:A:598:ASP:OD1	1:A:797:GLU:HA	2.10	0.50
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.94	0.50
4:A:8013:DMS:H12	5:A:4661:HOH:O	2.11	0.50
1:D:361:PRO:HB2	1:D:576:ILE:HG12	1.93	0.50
1:C:1021:CYS:HB2	5:C:4910:HOH:O	2.11	0.50
1:D:379:MET:HE1	1:D:387:VAL:HB	1.94	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.94	0.50
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.49
1:A:573:GLN:HB2	1:A:602:CYS:O	2.12	0.49
1:A:724:GLU:O	1:B:847:LYS:NZ	2.45	0.49
1:D:653:HIS:CD2	1:D:701:VAL:HG21	2.46	0.49
1:A:88:SER:HA	1:A:366:VAL:HG21	1.94	0.49
1:A:755:ARG:HB3	1:A:769:TRP:HB2	1.94	0.48
1:C:576:ILE:HD12	4:C:8010:DMS:O	2.13	0.48
1:D:127:PHE:HE1	1:D:184:LEU:HG	1.78	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.64	0.48
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.78	0.48
1:B:794:GLY:HA3	5:B:4316:HOH:O	2.13	0.48
1:A:19:PRO:HD3	1:A:112:PRO:HB3	1.95	0.48
1:A:887:GLN:NE2	1:A:980:GLU:O	2.46	0.48
1:A:430:PRO:HG3	4:D:8014:DMS:H21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:ARG:HB3	1:C:769:TRP:HB2	1.96	0.48
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.49	0.47
1:A:561:ARG:HD3	1:B:525:SER:O	2.14	0.47
1:A:794:GLY:HA2	5:A:4309:HOH:O	2.15	0.47
1:D:768:MET:HE1	1:D:1020:TRP:CH2	2.48	0.47
1:B:88:SER:HA	1:B:366:VAL:HG21	1.95	0.47
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.47
1:B:216:HIS:CE1	4:B:8023:DMS:H23	2.50	0.47
1:B:653:HIS:CE1	1:B:667:GLU:HG2	2.50	0.47
1:C:794:GLY:HA3	5:C:4339:HOH:O	2.15	0.47
1:D:380:LYS:O	4:D:8003:DMS:H11	2.15	0.47
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.97	0.46
1:D:244:VAL:HG21	1:D:256:VAL:HG11	1.96	0.46
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.46
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.46
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.51	0.46
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.97	0.46
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.51	0.46
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.98	0.46
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.97	0.45
1:D:40:GLU:OE2	1:D:43:ARG:NH2	2.47	0.45
1:B:370:GLN:HB2	5:B:4876:HOH:O	2.14	0.45
1:C:451:PRO:HA	4:C:8001:DMS:H23	1.97	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.51	0.45
1:B:44:THR:OG1	1:B:46:ARG:HG3	2.16	0.45
1:B:750:GLU:HG2	1:B:755:ARG:HG3	1.99	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.70	0.45
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.51	0.45
1:A:546:LEU:HA	5:A:4126:HOH:O	2.17	0.45
1:B:629:PHE:O	4:B:8020:DMS:H12	2.17	0.45
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.99	0.45
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.99	0.45
1:D:427:THR:HG21	1:D:462:SER:HB3	1.98	0.45
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.98	0.45
1:D:262:GLN:NE2	1:D:299:LYS:HE3	2.31	0.45
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.99	0.45
1:D:625:GLN:NE2	5:D:4225:HOH:O	2.49	0.45
1:D:794:GLY:HA3	5:D:4324:HOH:O	2.16	0.45
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.51	0.44
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.43	0.44
1:B:320:GLY:HA2	4:B:8006:DMS:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLY:HA2	1:B:386:ALA:O	2.17	0.44
1:D:225:PHE:HA	1:D:243:GLU:O	2.18	0.44
1:D:478:VAL:HG21	4:D:8014:DMS:H12	1.99	0.44
1:C:93:HIS:CG	4:C:8012:DMS:H12	2.52	0.44
1:C:714:ILE:HG21	4:C:8013:DMS:H12	1.99	0.44
1:D:653:HIS:HD2	1:D:701:VAL:CG2	2.30	0.44
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.99	0.44
1:B:428:ASP:O	4:B:8013:DMS:H12	2.18	0.44
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.53	0.44
1:A:991:MET:HE3	1:A:1003:VAL:HG21	2.00	0.44
1:C:36:TRP:HH2	4:C:8004:DMS:H23	1.83	0.44
1:A:240:LEU:C	1:A:240:LEU:HD23	2.43	0.43
1:A:140:ARG:HG2	1:A:215:LEU:HB3	1.98	0.43
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.52	0.43
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.99	0.43
1:B:595:THR:HA	1:B:596:PRO:C	2.42	0.43
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.53	0.43
1:A:437:SER:O	1:A:441:THR:HG23	2.19	0.43
1:B:361:PRO:HB2	1:B:576:ILE:HG12	2.01	0.43
1:B:755:ARG:NH1	5:B:5110:HOH:O	2.52	0.43
1:B:200:GLN:HB2	1:B:202:MET:HE2	2.00	0.43
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.01	0.43
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.00	0.43
1:A:230:ARG:HG2	5:A:4748:HOH:O	2.18	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.42
1:A:595:THR:HA	1:A:596:PRO:C	2.45	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42
1:A:335:VAL:HG22	1:A:344:LEU:HD12	2.02	0.42
1:C:595:THR:HA	1:C:596:PRO:C	2.44	0.42
1:A:390:SER:HA	1:A:391:HIS:HA	1.76	0.42
1:D:478:VAL:CG2	4:D:8014:DMS:H12	2.49	0.42
1:D:508:GLU:OE2	4:D:8006:DMS:H11	2.20	0.42
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.55	0.42
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.42
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.54	0.42
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.49	0.42
1:B:390:SER:HA	1:B:391:HIS:HA	1.86	0.42
1:A:9:VAL:HG12	1:D:9:VAL:HG12	2.02	0.41
1:B:379:MET:HE1	1:B:387:VAL:HB	2.01	0.41
1:D:763:GLY:HA3	1:D:822:LEU:HD13	2.01	0.41
1:C:573:GLN:HB2	1:C:602:CYS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.50	0.41
1:A:708:TRP:CZ2	4:A:8003:DMS:H23	2.55	0.41
1:A:802:ASP:HA	1:A:803:PRO:HD2	1.97	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.92	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.70	0.41
1:C:714:ILE:HD12	4:C:8013:DMS:H23	2.02	0.41
1:D:699:ARG:HH11	1:D:714:ILE:HG21	1.86	0.41
1:C:525:SER:O	1:D:561:ARG:HD3	2.20	0.41
1:D:373:VAL:O	1:D:377:LEU:HG	2.20	0.41
1:A:367:MET:HA	1:A:367:MET:HE2	2.01	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.87	0.41
4:A:8004:DMS:O	4:A:8016:DMS:H21	2.20	0.41
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.55	0.41
1:D:88:SER:HA	1:D:366:VAL:HG21	2.02	0.41
1:B:795:VAL:HG13	1:B:797:GLU:O	2.21	0.41
1:B:755:ARG:HB3	1:B:769:TRP:HB2	2.02	0.41
1:A:45:ASP:O	4:A:8016:DMS:H23	2.20	0.40
1:A:628:GLN:NE2	4:A:8002:DMS:O	2.49	0.40
1:C:143:PHE:O	1:C:168:PRO:HA	2.22	0.40
1:C:246:MET:C	1:C:246:MET:SD	3.05	0.40
1:B:19:PRO:HD3	1:B:112:PRO:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1013/1052 (96%)	981 (97%)	32 (3%)	0	100	100
1	B	1013/1052 (96%)	980 (97%)	32 (3%)	1 (0%)	48	43
1	C	1013/1052 (96%)	985 (97%)	27 (3%)	1 (0%)	48	43
1	D	1013/1052 (96%)	976 (96%)	37 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4052/4208 (96%)	3922 (97%)	128 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	736	ALA
1	B	752	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	867/897 (97%)	863 (100%)	4 (0%)	81	85
1	B	867/897 (97%)	859 (99%)	8 (1%)	70	75
1	C	867/897 (97%)	860 (99%)	7 (1%)	73	77
1	D	867/897 (97%)	860 (99%)	7 (1%)	73	77
All	All	3468/3588 (97%)	3442 (99%)	26 (1%)	76	80

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	546	LEU
1	A	672	VAL
1	A	744	GLU
1	B	80	GLU
1	B	344	LEU
1	B	546	LEU
1	B	652	LEU
1	B	672	VAL
1	B	761	GLN
1	B	774	LYS
1	B	876	THR
1	C	344	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	546	LEU
1	C	672	VAL
1	C	795	VAL
1	C	817	GLN
1	C	876	THR
1	C	956	GLN
1	D	80	GLU
1	D	344	LEU
1	D	546	LEU
1	D	672	VAL
1	D	685	LEU
1	D	744	GLU
1	D	986	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	294	ASN
1	A	485	GLN
1	A	693	GLN
1	A	702	GLN
1	B	128	ASN
1	B	266	GLN
1	B	485	GLN
1	B	554	GLN
1	B	702	GLN
1	B	824	GLN
1	B	903	GLN
1	B	1017	GLN
1	B	1022	GLN
1	C	12	GLN
1	C	266	GLN
1	C	297	ASN
1	C	485	GLN
1	C	554	GLN
1	C	646	HIS
1	C	653	HIS
1	C	702	GLN
1	C	817	GLN
1	C	885	ASN
1	D	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	262	GLN
1	D	266	GLN
1	D	485	GLN
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	718	GLN
1	D	977	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 23 are monoatomic - leaving 78 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DMS	B	8003	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
4	DMS	A	8012	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
4	DMS	B	8008	-	3,3,3	2.80	1 (33%)	3,3,3	0.62	0
4	DMS	A	8010	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
4	DMS	C	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8013	-	3,3,3	2.70	1 (33%)	3,3,3	0.62	0
4	DMS	C	8005	-	3,3,3	2.65	1 (33%)	3,3,3	0.43	0
4	DMS	A	8019	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
4	DMS	B	8012	-	3,3,3	2.76	1 (33%)	3,3,3	0.66	0
4	DMS	C	8013	-	3,3,3	2.74	1 (33%)	3,3,3	0.74	0
4	DMS	D	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
4	DMS	A	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
4	DMS	C	8002	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
4	DMS	B	8021	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
4	DMS	C	8003	-	3,3,3	2.64	1 (33%)	3,3,3	0.26	0
4	DMS	C	8004	-	3,3,3	2.70	1 (33%)	3,3,3	0.66	0
4	DMS	C	8016	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
4	DMS	B	8023	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
4	DMS	B	8005	-	3,3,3	2.70	1 (33%)	3,3,3	0.29	0
4	DMS	D	8009	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
4	DMS	D	8010	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
4	DMS	B	8016	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
4	DMS	D	8005	-	3,3,3	2.62	1 (33%)	3,3,3	0.31	0
4	DMS	D	8012	-	3,3,3	2.70	1 (33%)	3,3,3	0.69	0
4	DMS	C	8014	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
4	DMS	B	8015	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
4	DMS	B	8006	-	3,3,3	2.70	1 (33%)	3,3,3	0.66	0
4	DMS	B	8011	-	3,3,3	2.71	1 (33%)	3,3,3	0.58	0
4	DMS	B	8017	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
4	DMS	B	8020	-	3,3,3	2.90	1 (33%)	3,3,3	0.78	0
4	DMS	A	8007	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
4	DMS	A	8001	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
4	DMS	B	8010	-	3,3,3	2.61	1 (33%)	3,3,3	0.34	0
4	DMS	A	8015	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
4	DMS	C	8019	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
4	DMS	A	8005	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
4	DMS	D	8003	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
4	DMS	C	8008	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
4	DMS	B	8022	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
4	DMS	A	8021	-	3,3,3	2.70	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	8004	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
4	DMS	B	8014	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
4	DMS	B	8002	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
4	DMS	D	8007	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
4	DMS	D	8001	-	3,3,3	2.71	1 (33%)	3,3,3	0.86	0
4	DMS	A	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
4	DMS	D	8013	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
4	DMS	C	8017	-	3,3,3	2.67	1 (33%)	3,3,3	0.40	0
4	DMS	B	8019	-	3,3,3	2.76	1 (33%)	3,3,3	0.61	0
4	DMS	C	8010	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
4	DMS	D	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
4	DMS	A	8020	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
4	DMS	C	8012	-	3,3,3	2.65	1 (33%)	3,3,3	0.62	0
4	DMS	A	8009	-	3,3,3	2.75	1 (33%)	3,3,3	0.66	0
4	DMS	A	8022	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
4	DMS	B	8007	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
4	DMS	B	8001	-	3,3,3	2.58	1 (33%)	3,3,3	0.45	0
4	DMS	B	8009	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
4	DMS	C	8001	-	3,3,3	2.70	1 (33%)	3,3,3	0.91	0
4	DMS	A	8016	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
4	DMS	D	8011	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
4	DMS	C	8018	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
4	DMS	C	8006	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
4	DMS	A	8018	-	3,3,3	2.68	1 (33%)	3,3,3	0.46	0
4	DMS	A	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
4	DMS	A	8008	-	3,3,3	2.76	1 (33%)	3,3,3	0.52	0
4	DMS	D	8014	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
4	DMS	D	8008	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
4	DMS	C	8020	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
4	DMS	B	8004	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
4	DMS	C	8011	-	3,3,3	2.67	1 (33%)	3,3,3	0.24	0
4	DMS	A	8013	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
4	DMS	D	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.57	0
4	DMS	A	8011	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
4	DMS	C	8015	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	C	8009	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
4	DMS	B	8018	-	3,3,3	2.71	1 (33%)	3,3,3	0.49	0
4	DMS	A	8017	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8020	DMS	O-S	4.87	1.82	1.50
4	B	8008	DMS	O-S	4.71	1.81	1.50
4	B	8012	DMS	O-S	4.63	1.80	1.50
4	A	8008	DMS	O-S	4.62	1.80	1.50
4	D	8008	DMS	O-S	4.62	1.80	1.50
4	A	8009	DMS	O-S	4.61	1.80	1.50
4	B	8021	DMS	O-S	4.61	1.80	1.50
4	B	8019	DMS	O-S	4.61	1.80	1.50
4	D	8006	DMS	O-S	4.60	1.80	1.50
4	B	8022	DMS	O-S	4.60	1.80	1.50
4	A	8017	DMS	O-S	4.60	1.80	1.50
4	A	8012	DMS	O-S	4.60	1.80	1.50
4	A	8015	DMS	O-S	4.59	1.80	1.50
4	C	8007	DMS	O-S	4.59	1.80	1.50
4	C	8008	DMS	O-S	4.59	1.80	1.50
4	A	8016	DMS	O-S	4.58	1.80	1.50
4	C	8013	DMS	O-S	4.57	1.80	1.50
4	A	8019	DMS	O-S	4.57	1.80	1.50
4	D	8014	DMS	O-S	4.57	1.80	1.50
4	B	8009	DMS	O-S	4.57	1.80	1.50
4	A	8020	DMS	O-S	4.57	1.80	1.50
4	A	8006	DMS	O-S	4.56	1.80	1.50
4	C	8009	DMS	O-S	4.56	1.80	1.50
4	B	8018	DMS	O-S	4.56	1.80	1.50
4	D	8007	DMS	O-S	4.56	1.80	1.50
4	A	8007	DMS	O-S	4.56	1.80	1.50
4	C	8019	DMS	O-S	4.55	1.80	1.50
4	C	8015	DMS	O-S	4.55	1.80	1.50
4	B	8011	DMS	O-S	4.55	1.80	1.50
4	D	8010	DMS	O-S	4.55	1.80	1.50
4	C	8020	DMS	O-S	4.55	1.80	1.50
4	A	8022	DMS	O-S	4.54	1.80	1.50
4	C	8016	DMS	O-S	4.54	1.80	1.50
4	B	8023	DMS	O-S	4.54	1.80	1.50
4	B	8005	DMS	O-S	4.54	1.80	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8018	DMS	O-S	4.54	1.80	1.50
4	B	8006	DMS	O-S	4.54	1.80	1.50
4	B	8013	DMS	O-S	4.54	1.80	1.50
4	D	8001	DMS	O-S	4.54	1.80	1.50
4	C	8001	DMS	O-S	4.53	1.80	1.50
4	A	8013	DMS	O-S	4.53	1.80	1.50
4	A	8011	DMS	O-S	4.53	1.80	1.50
4	D	8012	DMS	O-S	4.53	1.80	1.50
4	A	8021	DMS	O-S	4.53	1.80	1.50
4	C	8006	DMS	O-S	4.53	1.80	1.50
4	C	8004	DMS	O-S	4.52	1.80	1.50
4	D	8013	DMS	O-S	4.52	1.80	1.50
4	B	8016	DMS	O-S	4.52	1.80	1.50
4	A	8003	DMS	O-S	4.52	1.80	1.50
4	B	8014	DMS	O-S	4.51	1.80	1.50
4	A	8004	DMS	O-S	4.51	1.80	1.50
4	C	8014	DMS	O-S	4.51	1.80	1.50
4	B	8003	DMS	O-S	4.51	1.80	1.50
4	D	8011	DMS	O-S	4.51	1.80	1.50
4	B	8002	DMS	O-S	4.50	1.79	1.50
4	C	8017	DMS	O-S	4.50	1.79	1.50
4	B	8004	DMS	O-S	4.50	1.79	1.50
4	A	8002	DMS	O-S	4.50	1.79	1.50
4	D	8003	DMS	O-S	4.50	1.79	1.50
4	C	8011	DMS	O-S	4.49	1.79	1.50
4	A	8018	DMS	O-S	4.49	1.79	1.50
4	B	8007	DMS	O-S	4.49	1.79	1.50
4	C	8010	DMS	O-S	4.48	1.79	1.50
4	A	8010	DMS	O-S	4.48	1.79	1.50
4	C	8003	DMS	O-S	4.48	1.79	1.50
4	D	8009	DMS	O-S	4.47	1.79	1.50
4	B	8017	DMS	O-S	4.47	1.79	1.50
4	B	8015	DMS	O-S	4.46	1.79	1.50
4	C	8012	DMS	O-S	4.43	1.79	1.50
4	D	8004	DMS	O-S	4.43	1.79	1.50
4	C	8005	DMS	O-S	4.43	1.79	1.50
4	A	8001	DMS	O-S	4.42	1.79	1.50
4	C	8002	DMS	O-S	4.42	1.79	1.50
4	D	8005	DMS	O-S	4.40	1.79	1.50
4	B	8010	DMS	O-S	4.39	1.79	1.50
4	D	8002	DMS	O-S	4.39	1.79	1.50
4	A	8005	DMS	O-S	4.38	1.79	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8001	DMS	O-S	4.32	1.78	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8007	DMS	1	0
4	B	8013	DMS	1	0
4	C	8005	DMS	1	0
4	C	8013	DMS	2	0
4	D	8004	DMS	1	0
4	A	8002	DMS	1	0
4	C	8003	DMS	1	0
4	C	8004	DMS	1	0
4	B	8023	DMS	1	0
4	D	8012	DMS	1	0
4	C	8014	DMS	1	0
4	B	8006	DMS	1	0
4	B	8020	DMS	1	0
4	D	8003	DMS	2	0
4	A	8004	DMS	1	0
4	A	8003	DMS	1	0
4	D	8013	DMS	1	0
4	C	8010	DMS	1	0
4	D	8006	DMS	1	0
4	C	8012	DMS	1	0
4	C	8001	DMS	1	0
4	A	8016	DMS	2	0
4	D	8014	DMS	3	0
4	C	8020	DMS	1	0
4	A	8013	DMS	1	0
4	D	8002	DMS	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.13	62 (6%) 27 27	15, 27, 53, 86	0
1	B	1015/1052 (96%)	-0.28	40 (3%) 43 44	12, 21, 46, 88	0
1	C	1015/1052 (96%)	-0.30	33 (3%) 49 49	12, 22, 47, 89	0
1	D	1015/1052 (96%)	0.12	45 (4%) 39 39	15, 28, 53, 91	0
All	All	4060/4208 (96%)	-0.08	180 (4%) 39 39	12, 25, 51, 91	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	795	VAL	6.6
1	A	10	VAL	6.5
1	B	795	VAL	6.3
1	A	9	VAL	5.8
1	D	10	VAL	5.7
1	C	801	ILE	5.6
1	B	770	ILE	5.2
1	A	11	LEU	4.9
1	C	798	ALA	4.9
1	B	11	LEU	4.9
1	B	801	ILE	4.7
1	B	731	PRO	4.7
1	C	10	VAL	4.6
1	A	796	ALA	4.6
1	B	730	LEU	4.6
1	A	730	LEU	4.6
1	B	799	THR	4.5
1	D	795	VAL	4.5
1	C	11	LEU	4.4
1	D	76	CYS	4.4
1	B	9	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1023	LYS	4.3
1	C	9	VAL	4.3
1	A	795	VAL	4.2
1	B	10	VAL	4.2
1	A	180	GLY	4.2
1	D	9	VAL	4.2
1	D	129	VAL	4.2
1	B	771	GLY	4.1
1	B	685	LEU	4.1
1	D	730	LEU	4.1
1	C	770	ILE	4.1
1	D	801	ILE	4.1
1	D	685	LEU	4.1
1	A	76	CYS	4.0
1	A	798	ALA	3.9
1	B	732	ALA	3.9
1	B	733	ALA	3.9
1	A	799	THR	3.9
1	C	686	PRO	3.9
1	B	752	GLY	3.9
1	A	78	LEU	3.9
1	C	731	PRO	3.8
1	D	130	ASP	3.7
1	A	801	ILE	3.7
1	D	11	LEU	3.6
1	A	732	ALA	3.6
1	D	1022	GLN	3.6
1	B	1023	LYS	3.5
1	A	686	PRO	3.5
1	C	685	LEU	3.5
1	A	65	ALA	3.5
1	D	798	ALA	3.5
1	C	730	LEU	3.5
1	C	794	GLY	3.5
1	D	799	THR	3.5
1	D	687	GLN	3.4
1	D	796	ALA	3.4
1	A	685	LEU	3.4
1	C	1022	GLN	3.4
1	B	1022	GLN	3.3
1	C	699	ARG	3.3
1	C	733	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	127	PHE	3.3
1	D	731	PRO	3.2
1	B	753	ASN	3.2
1	A	79	PRO	3.2
1	D	686	PRO	3.2
1	A	85	VAL	3.2
1	B	800	ARG	3.2
1	B	729	THR	3.2
1	D	800	ARG	3.1
1	C	688	PRO	3.1
1	A	136	GLU	3.1
1	D	745	MET	3.1
1	C	799	THR	3.1
1	C	735	HIS	3.1
1	A	733	ALA	3.1
1	D	733	ALA	3.1
1	C	753	ASN	3.0
1	A	689	GLU	3.0
1	C	771	GLY	3.0
1	A	71	GLU	3.0
1	B	688	PRO	3.0
1	C	736	ALA	3.0
1	B	798	ALA	2.9
1	C	800	ARG	2.9
1	C	796	ALA	2.9
1	A	687	GLN	2.9
1	D	79	PRO	2.9
1	B	774	LYS	2.9
1	D	794	GLY	2.9
1	D	735	HIS	2.9
1	B	686	PRO	2.8
1	A	800	ARG	2.8
1	A	68	ALA	2.8
1	A	177	LEU	2.8
1	A	184	LEU	2.8
1	D	131	GLU	2.8
1	D	179	ALA	2.8
1	D	732	ALA	2.8
1	D	78	LEU	2.8
1	A	179	ALA	2.7
1	D	773	LYS	2.7
1	A	81	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	688	PRO	2.7
1	A	69	VAL	2.7
1	B	734	SER	2.7
1	D	689	GLU	2.6
1	A	734	SER	2.6
1	B	755	ARG	2.6
1	D	320	GLY	2.6
1	A	319	ASP	2.6
1	B	655	MET	2.6
1	A	16	TRP	2.6
1	A	158	TRP	2.6
1	B	794	GLY	2.6
1	A	735	HIS	2.6
1	B	773	LYS	2.6
1	C	689	GLU	2.5
1	A	84	VAL	2.5
1	A	77	ASP	2.5
1	B	71	GLU	2.5
1	A	63	PHE	2.5
1	A	94	GLY	2.5
1	A	129	VAL	2.5
1	D	12	GLN	2.5
1	B	12	GLN	2.5
1	B	687	GLN	2.5
1	A	62	TRP	2.5
1	A	130	ASP	2.4
1	C	772	ASP	2.4
1	C	732	ALA	2.4
1	C	774	LYS	2.4
1	B	736	ALA	2.4
1	B	796	ALA	2.4
1	C	12	GLN	2.4
1	A	155	ASN	2.3
1	B	772	ASP	2.3
1	D	737	ILE	2.3
1	A	181	GLU	2.3
1	A	175	ALA	2.3
1	D	699	ARG	2.3
1	A	149	ALA	2.3
1	A	431	ARG	2.3
1	D	655	MET	2.3
1	A	126	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	769	TRP	2.2
1	A	736	ALA	2.2
1	A	134	LEU	2.2
1	D	128	ASN	2.2
1	A	114	VAL	2.2
1	A	797	GLU	2.2
1	D	71	GLU	2.2
1	B	663	LEU	2.2
1	C	663	LEU	2.2
1	D	134	LEU	2.2
1	C	690	SER	2.2
1	A	731	PRO	2.1
1	A	117	GLU	2.1
1	D	634	GLN	2.1
1	D	736	ALA	2.1
1	B	76	CYS	2.1
1	A	1023	LYS	2.1
1	B	689	GLU	2.1
1	D	729	THR	2.1
1	A	72	SER	2.1
1	A	74	LEU	2.1
1	A	173	LEU	2.1
1	D	74	LEU	2.1
1	A	80	GLU	2.1
1	C	684	GLU	2.1
1	B	735	HIS	2.1
1	D	177	LEU	2.1
1	D	734	SER	2.1
1	A	83	THR	2.1
1	C	683	PRO	2.1
1	B	739	HIS	2.0
1	A	688	PRO	2.0
1	B	748	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	DMS	B	8012	4/4	0.50	0.33	108,109,109,111	0
4	DMS	B	8020	4/4	0.66	0.30	44,52,56,61	0
4	DMS	A	8009	4/4	0.68	0.35	89,90,90,92	0
4	DMS	A	8020	4/4	0.68	0.34	77,78,78,82	0
4	DMS	A	8017	4/4	0.75	0.30	71,72,74,75	0
4	DMS	B	8009	4/4	0.76	0.29	78,78,80,80	0
4	DMS	A	8012	4/4	0.77	0.30	88,88,89,91	0
4	DMS	A	8015	4/4	0.78	0.23	72,74,75,75	0
4	DMS	A	8013	4/4	0.78	0.32	66,69,69,70	0
4	DMS	C	8009	4/4	0.78	0.28	70,72,73,74	0
4	DMS	D	8006	4/4	0.78	0.26	75,77,79,82	0
4	DMS	B	8016	4/4	0.80	0.23	55,58,61,66	0
4	DMS	C	8016	4/4	0.81	0.23	61,61,64,65	0
4	DMS	D	8013	4/4	0.81	0.23	57,60,63,63	0
4	DMS	A	8016	4/4	0.82	0.24	68,69,71,72	0
4	DMS	C	8017	4/4	0.82	0.28	77,77,78,78	0
4	DMS	C	8019	4/4	0.83	0.21	60,60,65,70	0
4	DMS	B	8021	4/4	0.83	0.21	60,61,62,67	0
4	DMS	C	8013	4/4	0.83	0.22	43,47,49,56	0
4	DMS	A	8019	4/4	0.85	0.21	64,64,66,67	0
4	DMS	A	8006	4/4	0.85	0.20	62,62,64,70	0
4	DMS	D	8002	4/4	0.86	0.28	54,59,62,62	0
4	DMS	C	8004	4/4	0.86	0.21	44,46,52,53	0
4	DMS	D	8008	4/4	0.86	0.23	66,66,67,70	0
4	DMS	D	8009	4/4	0.86	0.20	49,51,52,55	0
4	DMS	D	8014	4/4	0.86	0.29	69,71,74,75	0
4	DMS	C	8011	4/4	0.87	0.22	51,54,57,58	0
4	DMS	C	8012	4/4	0.87	0.22	53,53,54,56	0
4	DMS	D	8011	4/4	0.87	0.22	72,72,74,75	0
4	DMS	A	8021	4/4	0.87	0.26	71,73,73,74	0
4	DMS	A	8018	4/4	0.88	0.21	64,65,65,65	0
3	NA	C	3104	1/1	0.88	0.11	35,35,35,35	0
4	DMS	B	8013	4/4	0.88	0.21	47,51,54,56	0
4	DMS	C	8007	4/4	0.89	0.21	53,54,59,62	0
4	DMS	C	8008	4/4	0.89	0.19	57,58,60,61	0
4	DMS	D	8001	4/4	0.89	0.19	42,45,48,52	0
2	MG	B	3002	1/1	0.89	0.11	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	3002	1/1	0.89	0.08	31,31,31,31	0
4	DMS	D	8007	4/4	0.89	0.20	52,53,53,55	0
4	DMS	A	8007	4/4	0.89	0.21	45,47,50,51	0
4	DMS	B	8022	4/4	0.89	0.19	49,52,53,53	0
3	NA	B	3103	1/1	0.89	0.13	48,48,48,48	0
4	DMS	D	8012	4/4	0.89	0.17	48,49,51,58	0
4	DMS	C	8006	4/4	0.89	0.21	56,58,61,61	0
4	DMS	D	8004	4/4	0.90	0.18	53,54,54,58	0
4	DMS	C	8014	4/4	0.90	0.21	53,55,56,56	0
4	DMS	A	8008	4/4	0.90	0.18	49,53,55,57	0
4	DMS	C	8020	4/4	0.90	0.18	50,52,52,55	0
4	DMS	C	8005	4/4	0.91	0.18	37,40,44,47	0
3	NA	A	3103	1/1	0.91	0.11	41,41,41,41	0
4	DMS	B	8023	4/4	0.91	0.19	58,59,61,61	0
4	DMS	B	8006	4/4	0.91	0.19	39,46,46,49	0
4	DMS	D	8005	4/4	0.92	0.17	43,45,49,49	0
4	DMS	C	8018	4/4	0.92	0.13	35,37,41,43	0
4	DMS	A	8004	4/4	0.92	0.15	53,54,55,59	0
4	DMS	B	8018	4/4	0.92	0.17	56,58,59,62	0
4	DMS	C	8001	4/4	0.92	0.15	28,33,39,40	0
4	DMS	C	8015	4/4	0.92	0.18	58,59,61,62	0
3	NA	C	3103	1/1	0.92	0.09	43,43,43,43	0
3	NA	D	3103	1/1	0.92	0.11	49,49,49,49	0
3	NA	B	3104	1/1	0.93	0.09	35,35,35,35	0
3	NA	D	3102	1/1	0.93	0.06	24,24,24,24	0
4	DMS	D	8010	4/4	0.93	0.15	51,54,56,57	0
4	DMS	A	8010	4/4	0.93	0.14	47,48,48,51	0
2	MG	A	3002	1/1	0.93	0.08	33,33,33,33	0
4	DMS	B	8014	4/4	0.93	0.16	50,53,54,57	0
2	MG	C	3001	1/1	0.94	0.05	17,17,17,17	0
4	DMS	A	8002	4/4	0.94	0.18	32,35,37,40	0
3	NA	D	3101	1/1	0.94	0.08	29,29,29,29	0
2	MG	B	3001	1/1	0.94	0.04	17,17,17,17	0
4	DMS	B	8015	4/4	0.94	0.17	41,42,45,55	0
4	DMS	A	8022	4/4	0.94	0.14	57,57,58,58	0
4	DMS	B	8017	4/4	0.94	0.12	38,40,41,43	0
4	DMS	B	8004	4/4	0.94	0.11	22,26,33,34	0
4	DMS	A	8011	4/4	0.94	0.14	50,51,53,56	0
4	DMS	C	8010	4/4	0.94	0.16	33,34,40,47	0
4	DMS	B	8008	4/4	0.94	0.14	38,43,45,46	0
4	DMS	B	8002	4/4	0.95	0.12	23,29,30,34	0
3	NA	C	3102	1/1	0.95	0.06	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	3101	1/1	0.95	0.05	29,29,29,29	0
3	NA	B	3102	1/1	0.95	0.06	21,21,21,21	0
4	DMS	B	8019	4/4	0.95	0.12	30,31,41,43	0
4	DMS	C	8002	4/4	0.95	0.11	30,31,36,41	0
2	MG	C	3002	1/1	0.96	0.08	21,21,21,21	0
4	DMS	D	8003	4/4	0.96	0.13	38,41,42,43	0
4	DMS	B	8011	4/4	0.96	0.11	44,45,46,49	0
2	MG	A	3001	1/1	0.96	0.05	24,24,24,24	0
4	DMS	B	8007	4/4	0.96	0.10	36,38,39,44	0
4	DMS	A	8003	4/4	0.96	0.11	36,36,39,42	0
2	MG	B	3007	1/1	0.97	0.05	46,46,46,46	0
4	DMS	A	8005	4/4	0.97	0.10	34,39,40,41	0
4	DMS	B	8005	4/4	0.97	0.09	34,37,37,38	0
4	DMS	B	8010	4/4	0.97	0.10	32,35,38,40	0
4	DMS	C	8003	4/4	0.97	0.10	34,38,39,41	0
3	NA	C	3101	1/1	0.97	0.05	23,23,23,23	0
3	NA	B	3101	1/1	0.98	0.04	20,20,20,20	0
3	NA	A	3102	1/1	0.98	0.03	17,17,17,17	0
4	DMS	A	8001	4/4	0.98	0.07	23,30,31,32	0
4	DMS	B	8001	4/4	0.98	0.07	22,26,27,29	0
2	MG	D	3001	1/1	0.98	0.03	20,20,20,20	0
4	DMS	B	8003	4/4	0.98	0.08	32,36,36,37	0

6.5 Other polymers

There are no such residues in this entry.